

Development of a Formalism of Discrete Element Method for Numerical Modeling of Fracture of Heterogeneous Elastic-Plastic Materials

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Abstract. A general approach to realization of models of elasticity, plasticity and fracture of heterogeneous materials within the framework of discrete element method (DEM) is proposed in the paper. It is based on building many-body forces of discrete element interaction, which provide response of element ensemble correctly conforming to the response of simulated solids. Developed formalism makes possible realization of various rheological models in the framework of DEM to study deformation and fracture of solid-phase media of various natures.

Introduction

An important direction in fracture mechanics is development of numerical methods and their application to study dynamics and peculiarities of fracture of heterogeneous materials and structures under complex loading conditions. A perspective and intensively developed representative of numerical methods used to solve fracture mechanics problems is a discrete element method (DEM) [1-2]. In the framework of “conventional” particle methods simulated material is considered as an ensemble of interacting particles (elements) having finite size and predefined initial shape that can change as a consequence of loading. Evolution of an ensemble is defined by solution of the system of Newton-Euler motion equations:

$$\begin{cases} m_i \frac{d^2 \vec{R}_i}{dt^2} = \sum_{j=1}^{N_i} (\vec{F}_n^{ij} + \vec{F}_\tau^{ij}) \\ \hat{J}_i \frac{d^2 \vec{\Theta}_i}{dt^2} = \sum_{j=1}^{N_i} \vec{M}_{ij} \end{cases}, \quad (1)$$

where \vec{R}_i and $\vec{\Theta}_i$ are radius-vector and rotation angle of the particle i , m_i and \hat{J}_i are particle mass and moment of inertia, \vec{F}_n^{ij} and \vec{F}_τ^{ij} are forces of central (normal) and tangential interaction of considered element i with neighbor j , \vec{M}_{ij} is momentum of force, N_i is a number of neighbors (conventionally only nearest neighbors of element i are taken into account).

A fundamental feature of the formalism of DEM is an inherent capability of discrete element to change surroundings (interacting neighbours). This allows considering *the DEM as an attractive numerical technique to be used for direct modeling multiple fracture* accompanied by formation and mixing of large number of fragments. Note that coupling (adhesion) of fragments can be included in the model as well. This capability is taken into account by means of change of the state of the pair of discrete elements (“linked” pair ↔ “unlinked” pair, Fig. 1).

In spite of described advantage, at present time field of application of DEM is limited mainly by study of deformation and fracture of brittle materials and weakly bonded media [1-3]. These limitations are concerned with insufficient development of mathematical models of interaction of discrete elements.

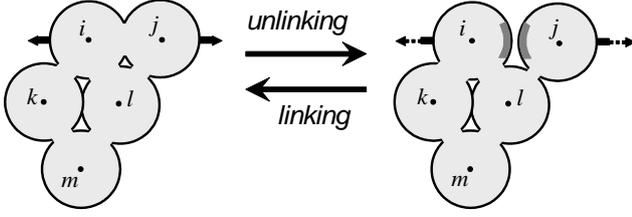


Fig.1. Schematic representation of switching between *linked* (at the left) and *unlinked* (at the right) states of the pair of discrete elements i and j .

Therefore one of fundamental problems in DEM is formulation of interaction potentials/forces (namely of \vec{F}_n^{ij} and \vec{F}_τ^{ij} in Eq. 1), which provide response of element ensemble conforming to response (including fracture) of consolidated solids with various rheological properties. An approach to solving this problem with use of *many-body interaction forces* is proposed in the present paper. The approach is realized within the framework of two-dimensional version of the movable cellular automaton (MCA) method [4-5], which integrates the possibilities of DEM and another discrete numerical technique, namely of cellular automaton method.

Formulation of discrete element interaction in many-body form

The main idea of proposed approach is to represent element interaction forces in the structural form with separated pair-wise and volume-dependent parts:

$$m_i \frac{d^2 \vec{R}_i}{dt^2} = \vec{F}_i = \sum_{j=1}^{N_i} \vec{F}_{pair}^{ij} + \vec{F}_\Omega^i, \quad (2)$$

where pair-wise constituents \vec{F}_{pair}^{ij} depend on spatial position/displacement of element i with respect to nearest neighbor j , volume-dependent constituent \vec{F}_Ω^i is concerned to combined influence of nearest surroundings of the element. When simulating locally isotropic medium the volume-dependent contribution can be expressed in terms of pressure P_i in the volume of discrete element i :

$$\vec{F}_\Omega^i = -A \sum_{j=1}^{N_i} P_i S_{ij} \vec{n}_{ij} \quad (3)$$

where S_{ij} is square of area of interaction (contact) of elements i and j , \vec{n}_{ij} is a unit vector directed along the line between mass centres of considered elements, A is a parameter. In such formulation the right part of the Eq. 2 can be divided into sum of central (\vec{F}_n^{ij}) and tangential (\vec{F}_τ^{ij}) constituents:

$$\vec{F}_i = \sum_{j=1}^{N_i} (\vec{F}_{pair}^{ij} - A P_i S_{ij} \vec{n}_{ij}) = \sum_{j=1}^{N_i} [(F_{pair,n}^{ij}(h_{ij}) - A P_i S_{ij}) \vec{n}_{ij} + F_{pair,\tau}^{ij}(l_{ij}^{shear}) \vec{t}_{ij}] = \sum_{j=1}^{N_i} (\vec{F}_n^{ij} + \vec{F}_\tau^{ij}), \quad (4)$$

where $F_{pair,n}^{ij}$ and $F_{pair,\tau}^{ij}$ are central and tangential components of pair-wise interaction force that depend on the values of element-element overlap h_{ij} and relative shear displacement l_{ij}^{shear} [5].

It is seen from Eq. 3 that an important problem of building many-particle interaction forces is definition of local value of pressure (P_i) in the volume of discrete element. This parameter can be calculated with use of diagonal components of average stress tensor $\bar{\sigma}_{\alpha\beta}^i$ in the volume of the element i ($P_i = -\bar{\sigma}_{mean}^i = -(\bar{\sigma}_{xx}^i + \bar{\sigma}_{yy}^i + \bar{\sigma}_{zz}^i)/3$). This tensor is defined through surface forces (forces F_n^{ij} and F_τ^{ij} of interaction of the element with surroundings). In the considered case of plane motion of three-dimensional objects (quasi-two-dimensional approximation) an expression connecting $\bar{\sigma}_{\alpha\beta}^i$ and interaction forces is written as follows [2,5]:

$$\bar{\sigma}_{\alpha\beta}^i = \frac{1}{V_i} \sum_{j=1}^{N_i} q_{ij} \left[F_n^{ij} \cos\theta_{ij,\alpha} \cos\theta_{ij,\beta} \pm F_\tau^{ij} \cos\theta_{ij,\alpha} \sin\theta_{ij,\beta} \right], \quad (5)$$

where $\alpha, \beta = x, y$ (XY is a plane of motion); V_i is a current value of the volume of element i ; q_{ij} is a distance from mass centre of element i to the central point of area of interaction (contact area) with neighbour j ; $\theta_{ij,\alpha}$ is an angle between the line connecting mass centres of interacting elements i and j and axis α of laboratory system of coordinates.

It follows from Eqs. 2-5 that element interaction forces F_n^{ij} and F_τ^{ij} are linearly concerned with local values of stress tensor components $\bar{\sigma}_{\alpha\beta}^i$ and are mutually integrated through pressure P_i . Analysis of these relationships leads to the conclusion that *expressions for forces of interaction of elements*, which model a medium with certain rheological characteristics, could be directly reformulated *from constitutive equations of modeled medium* (equations of state). Below is a derivation of such expressions for locally isotropic elastic-plastic materials.

Discrete element interaction for modeling elastic-plastic medium

Stress-strain state of isotropic linearly elastic medium is described on the basis of generalized Hooke's law. The following notation of this law will be used in the paper:

$$\begin{cases} \sigma_{\alpha\alpha} = 2G\varepsilon_{\alpha\alpha} + (1 - 2G/K)\sigma_{mean}, \\ \tau_{\alpha\beta} = G\gamma_{\alpha\beta} \end{cases}, \quad (6)$$

where $\alpha, \beta = x, y, z$; $\sigma_{\alpha\alpha}$ and $\varepsilon_{\alpha\alpha}$ are diagonal components of stress and strain tensors; $\tau_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ are off-diagonal components; $\sigma_{mean} = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$ is mean stress; K is bulk modulus; G is shear modulus. It is seen that the form and the matter of Eq. 6 for diagonal and off-diagonal stress tensor components are analogous to relations in right part of Eq. 4 describing connection between total and pair-wise parts of normal and tangential forces of interaction of discrete elements. This leads to the simple idea to write down expressions for force response of automaton i to the impact of the neighbor j by means of direct reformulation of Hooke's law relationships:

$$\begin{cases} \sigma_{ij} = F_n^{ij} / S_{ij} = 2G_i \varepsilon_{i(j)} + \left(1 - 2G_i / K_i\right) \bar{\sigma}_{mean}^i, \\ \tau_{ij} = F_\tau^{ij} / S_{ij} = 2G_i \gamma_{i(j)} \end{cases}, \quad (7)$$

where G_i and K_i are shear and bulk elastic moduli of material filling the element i , $\varepsilon_{i(j)}$ and $\gamma_{i(j)}$ are contributions of the element i to the total values of normal and shear strains of the pair $i-j$ ($\varepsilon_{i(j)} + \varepsilon_{j(i)} = h_{ij} / r_{ij}^0$ and $\gamma_{i(j)} + \gamma_{j(i)} = l_{ij}^{shear} / r_{ij}^0$; r_{ij}^0 is initial distance between mass centers of elements i and j), mean stress $\bar{\sigma}_{mean}^i$ is calculated using Eq. 5. Note that proposed Eq. 7 for force of element response to the impact of the neighbor j are well-founded. Thus, by substituting Eq. 7 in Eq. 5 it is easy to show that proposed expressions for respond force automatically provide implementation of Hooke's law for components of average stress ($\bar{\sigma}_{\alpha\beta}^i$) and strain ($\bar{\varepsilon}_{\alpha\beta}^i$) tensors in the volume of element i [5].

Proposed Eq. 7 make it possible to calculate central and tangential interaction of discrete elements, whose ensemble simulates isotropic elastic medium. Taking into account the need to implement Newton's third law for interacting pairs of discrete element ($\sigma_{ij} = \sigma_{ji}$ and $\tau_{ij} = \tau_{ji}$) and the need to

distribute element contributions to normal and shear strains of the pair i - j the expressions for specific interaction forces can be written as follows:

$$\begin{cases} \Delta\sigma_{ij} = \Delta\sigma_{ji} = 2G_i\Delta\varepsilon_{i(j)} + \left(1 - \frac{2G_i}{K_i}\right)\Delta\bar{\sigma}_{mean}^i = 2G_j\Delta\varepsilon_{j(i)} + \left(1 - \frac{2G_j}{K_j}\right)\Delta\bar{\sigma}_{mean}^j \\ \Delta\varepsilon_{i(j)} + \Delta\varepsilon_{j(i)} = \Delta h_{ij} / r_{ij}^0 \\ \Delta\tau_{ij} = \Delta\tau_{ji} = 2G_i\Delta\gamma_{i(j)} = 2G_j\Delta\gamma_{j(i)} \\ \Delta\gamma_{i(j)} + \Delta\gamma_{j(i)} = \Delta l_{ij}^{shear} / r_{ij}^0 \end{cases}, \quad (8)$$

Here, relations for calculating the central and tangential interaction forces are written in incremental fashion (in hypoelastic form).

It should be noted that in two-dimensional formulation of the problem approximations of plane stress or plane strain state are widely used. A similar approach is used in described model [5].

An important advantage of proposed approach to building many-body interaction of discrete elements is a capability to realize various models of elasticity and plasticity within the framework of different realization of DEM (including MCA method). In particular, a model of plastic flow (incremental plasticity) with the criterion of Mises was implemented to simulate deformation of isotropic elastic-plastic media. For this purpose, radial return algorithm of Wilkins [6] was adopted to discrete element approach. Being formulated in terms of stress, for components of average stress tensor in the volume of discrete element i it will take the following form (Fig. 2):

$$\left(\bar{\sigma}_{\alpha\beta}^i\right)' = \left(\bar{\sigma}_{\alpha\beta}^i - \delta_{\alpha\beta}\bar{\sigma}_{mean}^i\right)M_i + \delta_{\alpha\beta}\bar{\sigma}_{mean}^i, \quad (9)$$

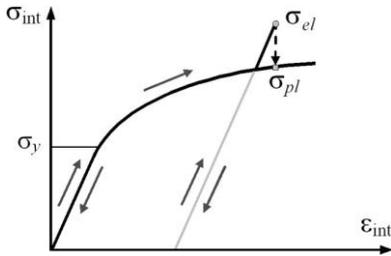


Fig.2. Schematic representation of functioning of radial return algorithm of Wilkins. Here σ_{el} is stress intensity after elastic problem solution at the current time step.

where $\alpha, \beta = x, y, z$; $\left(\bar{\sigma}_{\alpha\beta}^i\right)'$ are corrected (returned) average stress tensor components; $\bar{\sigma}_{\alpha\beta}^i$ are stress tensor components, which result from solution of elastic problem (Eq. 8) at the current time step; $\delta_{\alpha\beta}$ is the Kronecker delta; $M_i = \sigma_{pl}^i / \bar{\sigma}_{int}^i$ is current value of stress drop coefficient for discrete element i ; σ_{pl}^i is current radius of von Mises yield circle for the element i ; $\bar{\sigma}_{int}^i$ is stress intensity calculated with use of average stresses $\bar{\sigma}_{\alpha\beta}^i$ after solving elastic problem at the current time step.

By analogy with the elastic problem the expressions for correction of specific central and tangential forces of response of the element i (σ_{ij} and τ_{ij}) are derived by direct reformulation of Eq. 9 for average stresses:

$$\begin{cases} \sigma'_{ij} = \left(\sigma_{ij} - \bar{\sigma}_{mean}^i\right)M_i + \bar{\sigma}_{mean}^i \\ \tau'_{ij} = \tau_{ij}M_i \end{cases}, \quad (10)$$

where σ_{ij} and τ_{ij} are specific interaction forces, which result from solution of elastic problem at the current time step. It is easy to show that substitution of Eq. 10 in Eq. 5 for average stress tensor automatically provides reduction of its components to yield circle for the element i [5]. This demonstrates the correctness of the proposed model.

Note that independent use of the expressions Eq. 10 for interacting elements i and j can lead to

unequal values of respond forces ($\sigma'_{ij} \neq \sigma'_{ji}$ and $\tau'_{ij} \neq \tau'_{ji}$) in the pair i - j in case of different coefficients M_i and M_j and mean stresses $\bar{\sigma}_{mean}^i$ and $\bar{\sigma}_{mean}^j$. In view of the need for implementation of Newton's third law scaling of specific interaction force in each pair i - j has to be done with use of "unique" values of stress scaling coefficient M_{ij} and mean stress σ_{mean}^{ij} :

$$\begin{cases} M_{ij} = (M_i q_{ji} + M_j q_{ij}) / r_{ij} \\ \sigma_{mean}^{ij} = (\bar{\sigma}_{mean}^i q_{ji} + \bar{\sigma}_{mean}^j q_{ij}) / r_{ij} \end{cases}, \quad (11)$$

where r_{ij} is current distance between mass centers of elements i and j . As this takes place, scaling of forces of interaction of discrete elements i and j will take the following form:

$$\begin{cases} \sigma'_{ij} = (\sigma_{ij} - \sigma_{mean}^{ij}) M_{ij} + \sigma_{mean}^{ij} \\ \tau'_{ij} = \tau_{ij} M_{ij} \end{cases}. \quad (12)$$

In considered two-dimensional statement of the problem scaling of stress $\bar{\sigma}_{zz}^i$ is carried out with use of Eq. 10 with taking into account peculiarities for approximations of plane strain and plane stress state.

Testing results have shown that proposed model of elastic-plastic interaction of discrete elements provides good agreement of spatial distribution of stresses and strain in the ensemble of discrete elements modeling elastic-plastic medium with corresponding analytical solutions as well as with results of numerical simulation by means of commercial software ANSYS/LS-DYNA.

Calculation of fracture criteria in discrete element method

Potentialities of the developed approach to building many-body interaction of discrete elements make it possible to apply various *parametric "force" fracture criteria* (Huber-Mises-Hencky, Mohr-Coulomb, Drucker-Prager and so on) *within the formalism of DEM*. In DEM fracture is modeled by means of change of the state of the pair of discrete elements (transition from "linked" state of the pair to "unlinked" state with a possibility of further contact interaction of elements, Fig. 1). One of the ways of application of parametric fracture criteria as criteria of pair bond breaking is to determine local values of stress tensor components at the area of interaction (contact area) of considered pair i - j (hereinafter denote this tensor as $\sigma_{\alpha'\beta'}^{ij}$). In the local coordinate system $X'Y'$ of the pair (Fig. 3) components $\sigma_{y'y'}^{ij}$ and $\sigma_{x'y'}^{ij}$ for the pair i - j are numerically equal to specific forces of central (σ_{ij}) and tangential (τ_{ij}) interaction of the elements (these forces are applied to the contact area S_{ij}). Other components ($\sigma_{x'x'}^{ij}$ and $\sigma_{z'z'}^{ij}$) of stress tensor in the local coordinate system $X'Y'$ are defined on the basis of linear interpolation of corresponding values ($\bar{\sigma}_{x'x'}^i$ and $\bar{\sigma}_{x'x'}^j$, $\bar{\sigma}_{z'z'}^i$ and $\bar{\sigma}_{z'z'}^j$) for elements i and j to the area of interaction:

$$\begin{cases} \sigma_{x'x'}^{ij} = (\bar{\sigma}_{x'x'}^i q_{ji} + \bar{\sigma}_{x'x'}^j q_{ij}) / r_{ij} \\ \sigma_{z'z'}^{ij} = (\bar{\sigma}_{z'z'}^i q_{ji} + \bar{\sigma}_{z'z'}^j q_{ij}) / r_{ij} \end{cases}, \quad (13)$$

where $\bar{\sigma}_{\alpha'\beta'}^i$ and $\bar{\sigma}_{\alpha'\beta'}^j$ are components of average stress tensor in the volume of elements i and j in the local coordinate system of the pair.

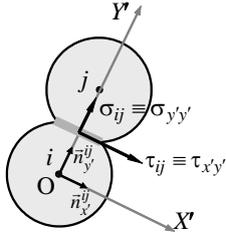


Fig.3. Instantaneous local coordinate system concerned with current spatial position of interacting pair i - j .

of stress tensor $\sigma_{\alpha'\beta'}^{ij}$.

Distinctive features of interaction of “unlinked” (i.e. contacting) elements i and j , among other things, are the lack of resistance to tension (pair is considered as interacting only when $\sigma_{ij} \leq 0$) and limited value of the force of tangential interaction. Maximum allowed value of tangential force (τ_{ij}) in “unlinked” pairs is determined by applied model of friction of surfaces of interacting elements (Amonton’s law of friction, model of Dieterich [7] and so on).

Study of crack growth dynamics with DEM

Testing of the developed formalism has shown its large potentiality to study problems connected with crack formation and development in solids. This can be demonstrated by the example of DEM-based numerical study of features of mode I (tensile) and mode II (shear) unstable crack propagation in brittle materials. In the framework of conventional fracture mechanics predictions a brittle crack cannot propagate faster than the Rayleigh wave speed V_R . Nevertheless recent researches including numerical as well as experimental studies have shown a possibility of faster propagation of shear cracks [8,9]. This problem was analyzed with use of above described models of element interaction and pair bond breaking.

Simulation results have shown that in mode I fracture two vortexes with opposite rotation directions are formed in the front of propagating crack bilaterally along crack propagation line (Fig. 4a). As is shown in Fig. 4a, back parts of vortexes are confined to the crack tip. Opposite rotation directions of vortexes provide for tensile deformation of the tip in the direction normal to the crack line. In linear elastic brittle material such vortexes propagate with near Raleigh speed V_R (or slower) that determines maximum possible velocity of mode I crack development (Fig. 4b).

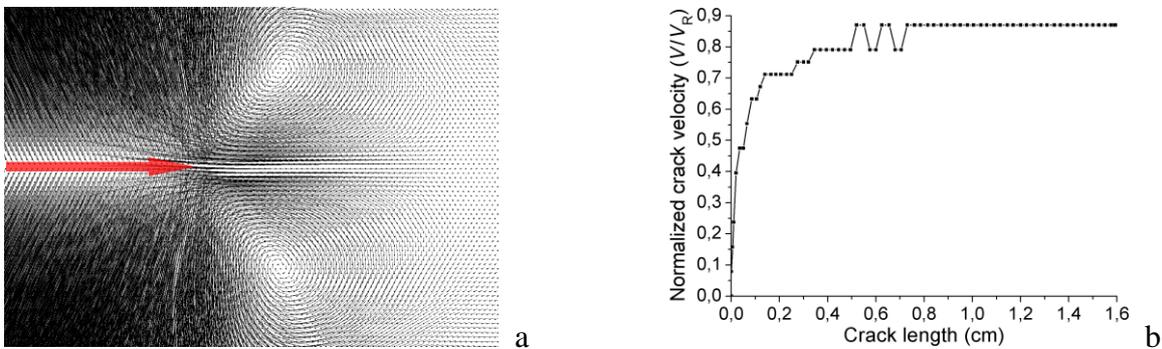


Fig.4. Velocity field near tip of mode I crack (a) and dependence of instantaneous values of crack velocity on crack length (b). Arrow in (a) shows crack line and propagation direction, arrow tip points to crack tip. Crack velocity V in (b) is normalized to Raleigh wave speed V_R .

Components $\sigma_{\alpha'\beta'}^{ij}$, thus defined, can be used to calculate necessary invariants of stress tensor which then can be used to calculate current value of applied criterion of pair fracture. In particular, below the examples of bond breaking conditions in the pair i - j with use of Huber-Mises-Hencky and Drucker-Prager criteria are shown:

$$\begin{cases} \sigma_{int}^{ij} > \sigma_c \\ \sigma_{int}^{ij} 0.5(a+1) + \sigma_{mean}^{ij} 1.5(a-1) > \sigma_c \end{cases} \quad (14)$$

where σ_c is corresponding threshold value for considered pair (value characterizing strength of chemical bond), a is a ratio of material compressive strength to tensile strength, σ_{int}^{ij} and σ_{mean}^{ij} are invariants

In case of mode II fracture at the initial stage of crack growth a vortex is formed in front of propagating crack. The center of vortex is situated in the vicinity of crack tip (Fig. 5a). As in mode I fracture, the maximum speed of vortex propagation in mode II is limited by Raleigh speed that determines limiting velocity of shear crack propagation. Nevertheless it is seen that in back part of the vortex velocity fields in lower and upper parts (with respect to crack line) are asymmetrical (Fig. 5a). In particular, velocities of elements near upper crack face in the vicinity of the crack tip are slightly larger than near lower crack face and therefore are oriented more vertically. Such asymmetry of velocity and displacement field near crack tip leads to asymmetry of stress distribution in front of growing crack. This asymmetry progressively increases with crack propagation and leads to stress concentration increase in front of the crack tip as well as to size increase of the area of peak stresses in front of crack. Therefore as crack grows, it steadily accelerates. Increasing asymmetry of velocity and displacement fields in front of the crack tip finally results in degradation of the local vortex and its transformation in area of local curvature of global longitudinal velocity field (Fig. 5b). Such kind of configuration of velocity field in the vicinity of crack tip provides for possibility of crack growth with velocities up to longitudinal elastic wave speed V_p . So, as crack propagates, its velocity continues to increase up to values close to V_p (Fig. 6a). Size of the area of peak stresses in front of the shear crack and stress concentration in this area becomes invariable as shear crack propagates with maximum velocity.

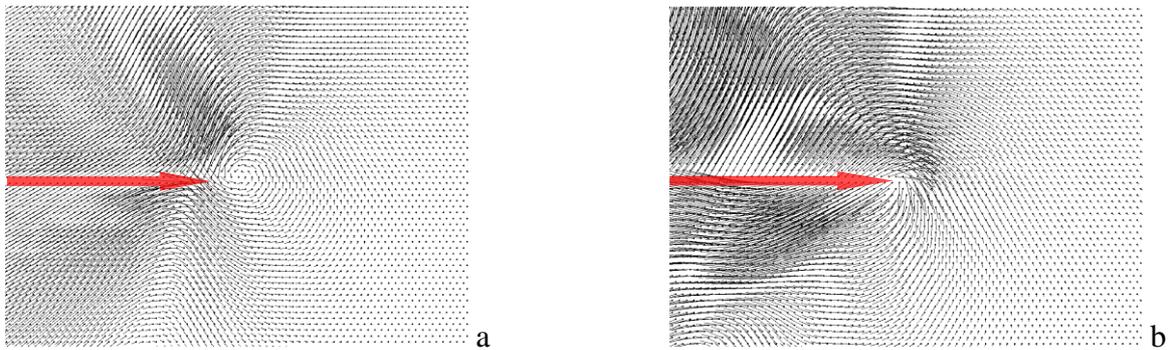


Fig.5. Velocity fields near tip of mode II crack at the stages of crack propagation with near-Raleigh velocity (a) and near-longitudinal wave velocity (b). Arrows show crack line and propagation direction, arrow tips point to crack tip.

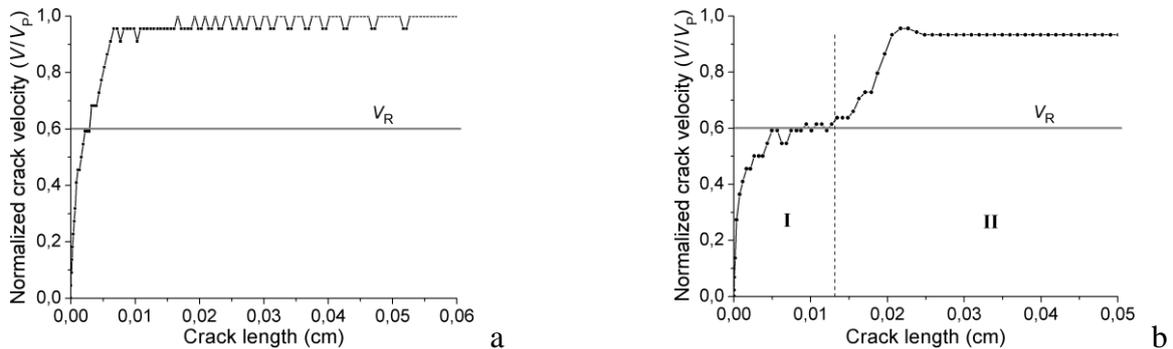


Fig.6. Dependences of instantaneous values of crack propagation velocity on crack length: a) crack develops from free surface; b) crack is initiated inside the sample far from free surfaces. Crack velocity V is normalized to longitudinal wave speed V_p .

Simulation results allowed authors to reveal peculiarities of mode II crack acceleration dynamics in cases of crack initiation at free surface and far from it (in the bulk of material). In the first case

nearly linear crack speed increase to maximum value takes place (Fig. 6a). In the second case (crack initiated under the condition of laminar shear deformation in the bulk of material) acceleration proceeds in two stages (Fig. 6b). At the first stage fast velocity increase to Raleigh speed V_R takes place. Then crack develops with this velocity for some time (area I in Fig. 6b). At the second stage crack velocity further increases to the limiting value close to longitudinal wave speed V_P and then becomes constant (area II in Fig. 6b). Described difference in dynamics of acceleration of incipient shear crack is concerned to the fact that near the free surface of the sample an area of global curvature is formed under the condition of shear deformation. This area is characterized by an increase in tangential stress up to a certain depth. Therefore a shear crack generated at free surface and growing inside the material initially propagates through an area of increasing tangential stresses. This provides for fast increase of crack velocity to maximum value. When shear crack is generated in the bulk of material, at the initial stage of crack development it forms such area of “global” curvature and then accelerates to maximum propagation velocity. Formation of this takes place gradually during the course of crack growth. This explains the achievement of the limiting value of the crack growth rate for large values of crack length (Fig. 6).

Summary

A solution to the problem of modeling the consolidated elastic-plastic media by ensemble of discrete elements is proposed in the paper. This solution is based on use of *many-particle interaction* forces and on determination of *volume-dependent constituent* of interaction via calculation of components of *average stress tensor* in the volume of discrete elements. Final relations for central and tangential interaction forces are derived from constitutive rheological equations for modeled medium. An important advantage of the proposed expressions for element interaction is a possibility of implementation of *various models of elastoplasticity or viscoelastoplasticity* (which are conventionally written in terms of stress/strain tensor components) in terms of element interaction force and displacement increments.

Another important advantage of the developed formalism of discrete element interaction is a possibility to directly apply *complex multiparametric fracture criteria* (Drucker-Prager, Mohr-Coulomb etc.) as *criteria of interelement bond breakage*. The use of these criteria is very important for correct modeling of fracture of complex heterogeneous materials of various nature.

At the present time described models of interaction of discrete elements are approved and widely applied to study *fracture-related problems* at different scales from nanoscopic to macroscopic one, *whose investigation by conventional numerical methods of continuum mechanics is difficult*. The problems of this type include, for example, physical and mechanical processes in contact patches of technical and natural frictional pairs [5,10], multiple (quasi-viscous) fracture of porous ceramics or composite coatings and so on.

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