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Kinetic approach to the development of computational dynamic models for brittle solids

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A B S T R A C T

The paper presents an approach to developing the mathematical formalism of the discrete element method to numerically study the inelastic behavior and fracture of brittle materials under dynamic loading. The approach adopts the basic principles of the kinetic theory of strength which postulate the finite time of nucleation of discontinuities and relaxation of local stresses in the material. A general methodology is proposed for constructing dynamic (kinetic) models of the mechanical behavior of a discrete element based on quasi-static models and using three dynamic material parameters (time parameters). The physical meaning of these parameters is discussed, and a method is proposed for estimating the magnitude of the parameters for a considered material using standard experimental data on its mechanical characteristics. The approach is verified by a dynamic formulation of two-parameter models of inelasticity and strength of brittle materials within the method of simply deformable discrete elements. The proposed way to the dynamic generalization of conventional quasi-static mechanical models is applicable to various Lagrangian numerical methods and makes it possible to numerically study the dynamic behavior features and to predict the mechanical characteristics of brittle materials at different strain rates (up to strain rates 10^3 s^{-1}) and different types of stress state.

1. Introduction

The macroscopic elastic, inelastic and strength properties of brittle materials are sensitive to the strain rate and can differ considerably from the mechanical behavior characteristics determined in quasi-static loading conditions [1–8]. In particular, a strong dependence of the strength and inelastic properties on the strain rate $\dot{\varepsilon}$ is observed in brittle materials within the range $\dot{\varepsilon} > 10^1$–10^2 s^{-1}. The effective elastic moduli of brittle materials change significantly at the strain rates $\dot{\varepsilon} > 10^3$ s^{-1}. Therefore, when constructing numerical mechanical behavior models for the most typical range of strain rates $\dot{\varepsilon} < 10^3$ s^{-1}, it is important to account for the effect of loading dynamics on the inelastic and strength properties of brittle materials.

The inelastic behavior of brittle materials is mainly associated with microdamage accumulation (formation of different-size voids and cracks, their growth or healing, coalescence, collapse, etc.) [9–11]. Lattice defects are involved in the deformation of such materials only at high pressures and temperatures [12]. Hence the dynamic inelastic behavior of brittle materials is generally described using modified plasticity models that account for the high sensitivity of inelastic response parameters to pressure, as well as the complex relationship between shear and volume plastic strains (non-associated flow rules) [13–20]. Noteworthy among them are the models that use the Drucker–Prager criterion and its modifications to describe inelastic deformation and fracture. Various implementations of these models are widely used to simulate the inelastic dynamic mechanical behavior of brittle solids [21–24].

Classical dynamic models use a conventional approach that accounts for the sensitivity of the inelastic behavior characteristics of the material to the change in the local strain rate. At the same time, the strain rate (in contrast to the physical mass velocity) is a technical parameter characterizing the volume-averaged rate of change in the dimensions of the specimen or its fragment. As a rule, integral values of $\dot{\varepsilon}$ for the entire specimen are used to determine experimentally the strain rate dependence of the parameters of the applied plasticity or fracture model. The local values of $\dot{\varepsilon}$ (e.g., in the region of crack nucleation) can differ significantly from the integral value in this case.

An alternative way of describing the inelastic deformation and fracture of dynamically loaded materials is the kinetic approach developed by Zhurkov [25], Regel [26], Bratov and Petrov [27], and Morozov and Petrov [28]. Within this approach, the process of the main crack nucleation and growth is characterized by a physical parameter

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called the fracture time. In the initial formulation of the kinetic theory, this parameter is associated with thermal fluctuations in the crystal lattice, and its magnitude is determined by the temperature and the applied load. Later it was shown that this physical parameter is scale dependent, and the hierarchy of the scales is related with the hierarchy of internal structural elements in the material [29–31]. Petrov and Morozov applied the kinetic approach to describe the conditions for the onset of inelastic deformation in the specimen or a fragment of the material. The proposed dynamic yield criterion takes into account the finite-time duration of the formation of a spatially distributed system of microdiscontinuities.

Significant progress in the kinetic approach has been made due to the introduction of the generalized concept of incubation time, which characterizes the time duration of the processes bringing about stress relaxation on the considered spatial scale [28,32,33]. The stress relaxation mechanisms can differ qualitatively for various relaxation processes (inelastic deformation, fracture) and various materials, but nevertheless these processes can be described within a general approach.

A widespread approach to studying the dynamic mechanical behavior of materials, including fracture, is numerical simulation in Lagrangian coordinates using explicit integration schemes [34–37]. Herewith, along with the conventional dynamic models of the inelastic mechanical behavior, the models based on the kinetic theory of strength become popular [38–40]. Continuum mechanics based numerical methods are conventionally used for the numerical study of the features of deformation of brittle materials under dynamic loading. The classical method of finite elements (FEM) and its extended formulations (including XFEM and PFEM) are the most popular representatives of this class of methods. We should also mention a novel formulation of FEM for brittle solids with discontinuities, namely, the dynamic phase field method [41–44]. However, in the last decade, “discrete” numerical methods have been actively used to solve dynamic problems. The simulated material in these methods is represented by an ensemble of interacting elements or particles of finite size and a certain shape that can change during deformation. An element is considered as a fragment of the material that can be cohesively/adhesively bonded to neighboring fragments, or be in contact, or not interact with them. Such methods are called discrete element methods (DEM) [45–49]. A key advantage of a discrete element is its ability to change the form of interaction with neighboring elements (linked, contact, unlinked), which provides the possibility to change its environment (the set of neighboring elements). This allows a direct simulation of such complex fracture processes as multiple cracking with crack branching, intensive mass transfer, and mixing of fragments [50–54]. Note that owing to the common formalism of various Lagrangian numerical methods (DEM, FEM [55–58], DEM + FEM [59,60], PFEM [61], XFEM [34]), general dynamic models of deformation and fracture of brittle materials can be constructed and implemented with regard to the capabilities of a particular method.

Despite the extensive use of discrete element methods for the numerical investigation of deformation and fracture of brittle heterogeneous materials, at present time the mathematical formalism of DEM is limited to conventional quasi-static models of the response of elements to mechanical loading (applicable at the characteristic strain rates $\dot{\varepsilon} < 10^1\ s^{-1}$). This restrains application of these very promising methods to the study of material behavior under high-rate loading. At the same time, DEM are advantageous for fracture simulation, first of all, for dynamically loaded brittle materials. To expand the applications of DEM for mechanical behavior analysis at high strain rates (including impact loading), rheological models are needed which take into account the dynamic response features of brittle materials.

In the present paper the new approach to development of dynamic models within the framework of the numerical Lagrangian discrete element method is proposed. The proposed approach uses the concept of the physical (kinetic) theory of strength for a general (dynamic) formulation of the conventional “quasi-static” yield and strength criteria with taking into account the finite times of local stress relaxation, damage and crack nucleation. The basic principles of constructing a “physical” model of the dynamic behavior of brittle materials are illustrated in this paper by the example of the movable cellular automata (MCA) method belonging to the group of methods of simply (homogeneously) deformable discrete elements [37,62,63]. Nikolaevsky's plasticity model of brittle solids [64,65] (non-associated plastic flow rule with the Mises–Schleicher yield criterion) and the model of failure with the Drucker–Prager criterion [66] are considered as generalizable quasi-static models of the inelastic response of discrete elements. It is shown that the proposed method of dynamic generalization of the discrete element formalism allows taking into account the deformation features of brittle solids at strain rates up to $\sim 10^3\ s^{-1}$. The approach is applicable to various representatives of Lagrangian numerical methods (including finite element and difference methods), and to various models and criteria of plasticity and strength of brittle materials.

2. The main approximations of the MCA method and the quasi-static model

The MCA method belongs to the family of “explicit” discrete element methods. The evolution of an ensemble of discrete elements in the explicit DEM is governed by an explicit numerical solution of the system of classical equations of motion [48]. The MCA method uses a widely accepted approximation of equivalent discs or spheres to interpret the element shape in the numerical solution of equations of motion (this enables the use of simplified Newton–Euler equations of motion) [47]. Within this approximation, the interaction between two discrete elements is divided into two independent contributions: central (oriented along the line connecting the centers of mass of the elements) and tangential (in the plane transverse to the mentioned line). The elements are assumed to interact if they have common edges/faces (i.e., two contacting equivalent discs/spheres). A consolidated fragment of a solid is modeled by assuming these contacts to be initially bonded. For damage/crack faces, such contacts are considered as unbonded [47,67].

The stress-strain state of a discrete element (movable cellular automaton) is described within the approximation of a homogeneous stress and strain distribution in the volume of the discrete element [48,68]. Stresses and strains in the discrete element are determined by the average stress tensor $\sigma_{\alpha\beta}$ and the average strain tensor $\varepsilon_{\alpha\beta}$. Components of the average stress tensor are calculated via surface forces, namely, by means of the forces of the element response to impacts of neighbors. A distinctive feature of the MCA implementation of DEM is the use of a many-body formulation of element-element interaction forces with the use of mean stresses and strains [37,62,63]. Hence the mean stresses/strain and the element-element interaction parameters (forces and relative displacements) are inextricably interrelated. This permits an easy implementation of various models of elasticity, plasticity (including models of inelastic behavior of brittle solids) and fracture, which are conventionally formulated in tensorial form [37,69]. A detailed description of the general statements of the MCA method is provided in the references [37,62,63] and sequentially stated in Supplementary Materials.

This paper considers a “dynamic generalization” of the discrete element implementation of quasi-static macroscopic models of plasticity and fracture of locally isotropic brittle materials (a discrete element is assumed to be filled with an isotropic material). Within a quasi-static model, the elastic response of an element to the mechanical action of neighboring elements is described on the basis of the linear Hooke's law [37,69]. A macroscopic plasticity model is used to describe damage-induced stress relaxation in an element beyond the yield point. In the paper we consider a popular model of the inelastic deformation response of brittle materials, such as Nikolaevsky's model (non-associated plastic flow rule). This model was chosen as an example because it adequately describes the response of a large group of brittle materials