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Fracture modeling with the discrete elements method

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Abstract. The discrete element method (DEM) is used to reveal the main features of fracture in materials with different degree of heterogeneity. It is shown that this method adequately describes the main properties of materials in the fracture process such as brittle and ductile behavior, two-staged nature of fracture in heterogeneous materials, heterogeneity of the spatial distribution of local internal stresses depending on the degree of material heterogeneity.

Keywords: materials fracture, Discrete Elements Method, heterogeneity

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Применение метода дискретных элементов для моделирования разрушения поликристаллических материалов

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Аннотация. Метод дискретных элементов применен для выявления закономерностей разрушения гетерогенных материалов. Показано, что модель адекватно описывает разрушение хрупких и пластичных материалов, двухстадийный характер разрушения гетерогенных материалов, а также неоднородность пространственного распределения внутренних локальных напряжений в зависимости от гетерогенности материала.

Ключевые слова: прочность и разрушение материалов, метод дискретных элементов

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Introduction

Fracture of materials remains to be the actual problem in connection with ongoing natural and technogenic catastrophes. At the same time, it is important to understand that fracture is not some kind of critical event that can be prevented by using materials with a safety margin or geometric dimensions with the ability to withstand the specified mechanical loads. On the contrary, fracture is a process evolving in space and time [1], and the parameters of materials, such as elastic moduli, local mechanical stresses and strains, structural rearrangements, and discontinuities, can undergo significant changes in this process. This process can be accompanied by various types of radiation (acoustic and electronic emission, mechanoluminescence), the parameters of which can serve as indicators or precursors of various kinds of events in the fracture process.

In contrast to the continual mechanics methods, the discrete element method (DEM) used in this work allows one to take into account explicitly the appearance of the local discontinuities during fracture process. We used the model of spherical particles (simulating polycrystalline grains) connected by bonds (simulating grain boundaries) located at the particle contacts. This bonded particle model (BPM) is described in detail in [2], and its various modifications are widely used to study the behavior of materials under mechanical load (for example, [3–8]). In the BPM model, the formation of cracks is determined by the breaking of bonds between particles, and their propagation is provided by the coalescence of many broken bonds [9].

The goal of this work was to study how the degree of materials heterogeneity influence the character of destruction and acoustic emission (AE) accompanying the fracture process. The breaking of a single bond was considered an elementary act of AE. Calculations were carried out in the freely distributed software package MUSEN [10]

Computer simulation

Cylindrical samples with a diameter of 10 mm and a height of 20 mm were modeled. The dimensions were selected in such a way that it was possible to compare the results obtained by computer modeling with the results of laboratory experiments obtained earlier on samples of the same dimensions. The cylinders were filled with spherical particles of the same or different radii and packed by the MUSEM packing generator until a porosity of 0.35–0.37 was reached. In this case, the overlap of the contacting spheres did not exceed 0.0001 mm.

Mechanical parameters of materials such as Young modules, Poisson ratios, normal and tangential strengths were set characteristic of rocks (quartz, orthoclase, oligoclase). We did not have a goal to compare values of the calculated strength of materials with their experimental strength, so the calibration of these parameters was not carried out. Two types of samples with different degrees of heterogeneity were used:

1. Homogeneous sample: grains (particles) and bonds with the properties of granite. The particle size was 0.4 mm, their number – 28125.

2. Grains (particles) with diameters obtained by a random number generator with a normal distribution (mean value of 0.3 mm and a standard deviation of 0.1 mm). Three types of particles (quartz, orthoclase, oligoclase) were generated with a percentage composition characteristic for granite; their number is 48695.

Bonds were formed at the places of particle contacts. Particles of the same material were connected by a bond from the matching material, and particles of different materials were connected either by low-strength brittle glass bonds (hereinafter referred to as the set of bonds type 1) or by low-modulus bonds [11] (hereinafter referred to as the set of bonds type 2). The bond diameter (d) was automatically chosen by the bond generator to be equal to the smaller diameter of the pair of connected particles 1 and 2: $d = \min\{d_1, d_2\}$ [10]. The maximum bond length (L_{max}) was chosen in such a way that one more particle could not fit between a pair of connected particles. The minimum length L_{min} was usually set to zero. It should be noted that with such a choice of L_{min}, the system can spontaneously explode, since

Fig 1. The sample and the simulation scheme

the overlap of particles mentioned above was allowed. If this happened, then the minimum bond length was taken equal to the maximum particle overlap (0.0001 mm) with the opposite sign.

The sample was placed in a virtual press, in which the lower plate was fixed, while the upper one descended at a speed of $v = 0.02$ m/s until the sample was destroyed (Fig. 1). Various mechanical parameters were recorded during the fracture process.

Results and Discussion

Figure 2 shows loading diagrams for samples of different heterogeneity and a homogeneous sample. The deformation was calculated using the formula $\varepsilon = \nu \cdot t$. Stress calculations were based on forces acting on the loading plates. Since in the numerical experiment it is generally impossible to maintain the equality of forces acting on the plates [12], the stress was calculated with the help of the formula $\sigma = 0.5\,(F_t + F_b)/S$, S is the initial cross section, indices t and b correspond to top and bottom.

One can see that more homogeneous samples (1 and 2 in Fig. 2, *a* and Fig. 2, *b*) are characterized by brittle behavior (linear increase in stress versus deformation) and a sharp decrease after reaching the maximum value. For more heterogeneous samples (curves 3–5 in Fig. 2, *a*), the presence of a nonlinear (plastic) stage in the loading diagram is observed. This is because weaker bonds break first, and only after that the strong ones.

The spatial inhomogeneity of bonds breakage is shown in Fig. 3. The sample was divided into 10 layers perpendicular to its height, and the fracture characteristics were calculated in each layer for each saved time point. Fig. 3, *a* shows the time dependence of the number of intact bonds averaged over layers (N) for the three samples under consideration: homogenous sample with the stress-strain curve on the Fig. 2, *b*, the sample with stress-strain curve 1 on the Fig. 2, a and the sample with the bonds of type 1 described above. Diameter of bonds in all these cases was 0.1 mm. Coefficient of variation (the ratio of N to its standard deviation) was chosen as a measure of spatial heterogeneity and is shown in Fig. 3, *b*.

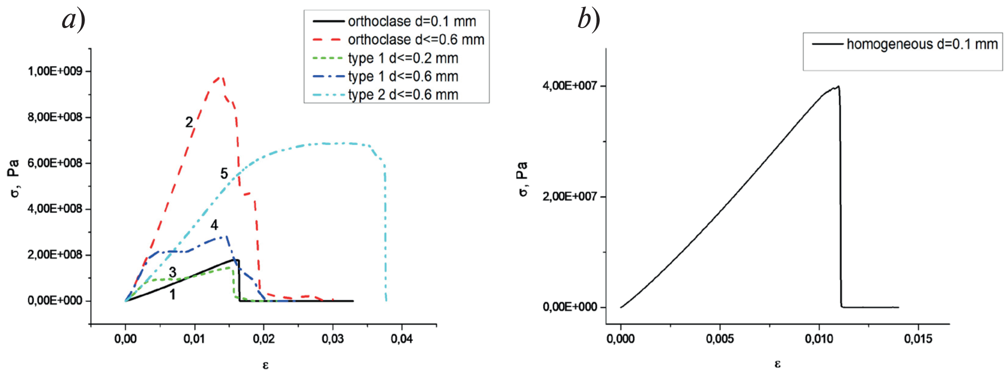

Fig. 2. Loading diagrams for samples with different types of bonds (*a*) and a homogeneous sample (*b*)

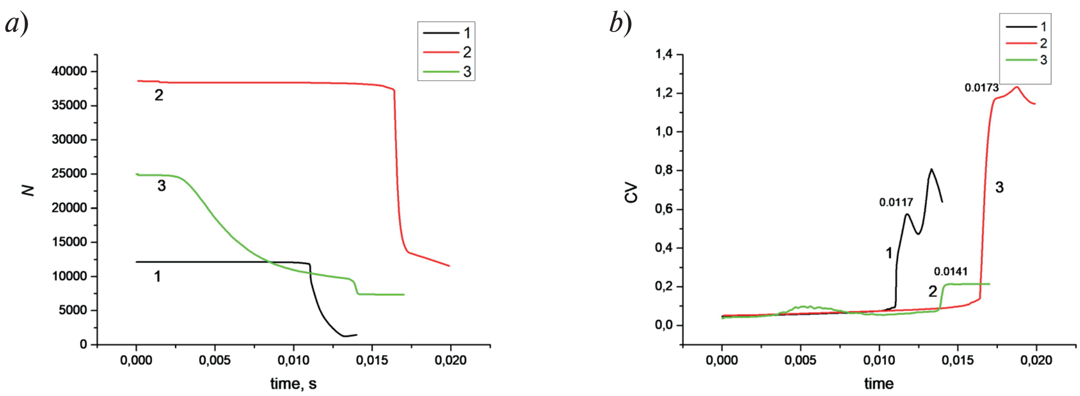

Fig. 3. Time dependence of the number of intact bonds averaged over the layers (*N*) (*a*) and the coefficient of variation (CV): 1 — homogeneous sample, 2 — sample with orthoclase bonds, 3 — sample with type 1 bonds (see text)

Brittle fracture is observed for samples 1 and 2: a negligible decrease in the number of intact bonds with a low coefficient of variation (spatial homogeneity) for quite a long simulation time and an after that, the rapid increase in CV close to the moment of destruction (localization of fracture and crack propagation). For heterogeneous sample 3, damage accumulates at much shorter times. However, the coefficient of variation at this stage is also small, which indicates that the damage accumulates more or less uniformly throughout the sample volume. This confirms the validity of the two-staged destruction model of heterogeneous materials proposed in [13, 14]. The rapid increase in the coefficient of variation is not very large too. This corresponds to the homogeneous nature of fracture in heterogeneous samples previously discovered in laboratory experiments [15], and a similar result obtained in the cellular automaton model [16].

For each layer, maximum tensile stresses acting on bonds σ_{max} were calculated. The reasons for the appearance of local tensile stresses under the action of an external compressive stress are well known (see, for example, [2]) and are not discussed here. Fig. 4, *a* shows the time dependences of the layer-averaged $\langle\sigma_{max}\rangle$ values. Fig. 4, *b* shows the time dependences of the coefficient of variation over the layers of the σ_{max} values.

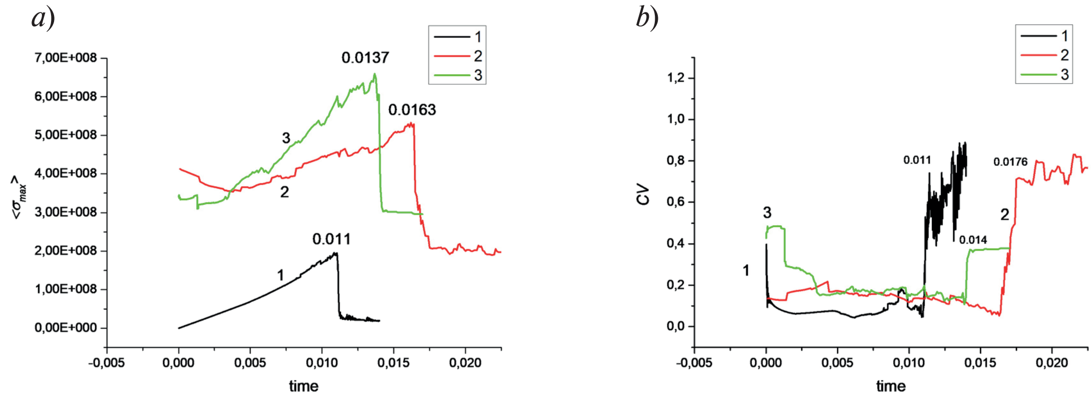

Fig. 4. Maximum tensile stresses averaged over layers (*a*) and their coefficients of variation (*b*): 1 – homogeneous sample, 2 – sample with orthoclase bonds, 3 – sample with type 1 bonds. The numbers on the graphs represent timestamps

In order to understand the time behavior of tensile stresses, one must keep in mind that the structure of grains and their boundaries (particles and bonds) created at the stage of material formation is not an equilibrium one and contains significant internal local stresses. At the initial stage of mechanical loading, these stresses relax. This relaxation time is so short compared to the characteristic loading time that it does not affect significantly the results obtained. This results in the nonmonotonicity of their time dependence at this stage (Fig. 4, *a*) and a significant coefficient of variation in Fig. 4, *b*. As stresses relax, they become more homogenous in the volume of the sample (Fig. 4, *b*) and increase in time (Fig. 4, *a*) until the conditions for the creation of a fracture center are formed. After this center is formed, local stresses again become significantly inhomogeneous in volume (Fig. 4, *b*). In a heterogeneous sample, the rate of this inhomogeneity is less than in samples that are more homogeneous.

Conclusion

The considered model of polycrystalline materials realistically describes some features of their destruction in cases where the main processes occur along grain boundaries. These features include the brittle nature of the destruction of homogeneous materials and the presence of nonlinear elasticity (plasticity) for more heterogeneous materials, revealed via the sigma-epsilon loading diagram (equation of state). For heterogeneous materials, the model predicts a two-stage nature of their fracture process, when at the first stage, the accumulation of defects occurs uniformly over the sample and at the second stage the formation and growth of the fracture center takes place.

The calculation of the maximum local stresses showed that the homogeneity of the material leads to greater spatial heterogeneity of local stresses and vice versa. The same behavior of local internal stresses calculated based on the kinetic concept of S.N. Zhurkov, was noted in laboratory experiments in [16].

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