The nonlinear relationship between local and macroscopic parameters of dynamic fracture in brittle composite materials

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Abstract. The paper describes results of a numerical study of the influence of composite structure parameters on the strength and fracture time of brittle materials under dynamic loading. The study is carried out on model concrete samples with different volume fractions of reinforcing inclusions and micropores. Simulation results show that the conventional principle of proportionality of the change in the incubation time of the fracture to the change in the linear dimensions of the fracture region is not applicable when a change in the spatial scale of the region is accompanied by a qualitative change in the parameters of the composite structure. The key factor determining the nonlinear nature of the change in the fracture incubation time during the transition from macroscale to lower scale representative volumes is the factor of phase interfaces, on which primary damage is predominantly localized. This conclusion is confirmed by much more pronounced dependence of the fracture time and dynamic strength of concrete samples on the quantitative concentration of inclusions (i.e. the characteristic distance between zirconia aggregates or micropores) than on volume fraction of inclusions.

1. Introduction

Traditional approaches to the structure design of multiphase (composite) materials and the estimation of critical stresses and strains under specified loading conditions are based on the use of mechanical characteristics of materials or phases obtained from static tests. At the same time, the material’s mechanical characteristics under dynamic impact may differ many times from the static ones [1-8]. This is of importance, first of all, for brittle materials. Macroscopic inelastic behavior of brittle solids results from the accumulation, growth, and merging of discontinuities (cracks) of various sizes. Since discontinuity formation is a time-distributed process, the discontinuities ensemble formation time is comparable with the characteristic loading time at high strain rates (> 10^2 s^-1) and cannot, therefore, be considered as negligible value. The maximum stress value in the material, in this case, is determined by the evolution dynamics of the discontinuities ensemble. This is especially relevant for composite materials in which interfaces between components play a decisive role in the formation of a discontinuities ensemble.

Such features of the dynamic mechanical behavior of brittle materials must be taken into account in analytical and numerical models used in the composite material design. This work aims to study the influence of structural features of brittle composite materials on their “integral” strength characteristics, including fracture time. The study was done by numerical modeling using the original model of the dynamic mechanical behavior of brittle solids [9,10] implemented within the numerical method of homogeneously deformable discrete elements (this method has a special name the method
of movable cellular automata) [11,12]. The model is based on the principles of the kinetic theory of strength [13-15] and takes into account the dynamics of the formation of a discontinuities ensemble in the bulk of the brittle material. We considered zirconium alumina concrete (ZAC), which is a typical brittle composite material. Note that ZAC is widely used as a material for structural elements of nuclear reactors (traps for corium released during accidents at nuclear power plants).

2. Model description

Mesoscale concrete samples were modeled with explicit taking into account the elements of the composite structure at the considered scale. The samples consist of a cement matrix containing particulate ZrO$_2$ inclusions. The volume fraction of inclusions ranged from 10% to 50%. Two types of aggregates in ZAC were taken into account: 1) large aggregates, which are angular particles of zirconium dioxide with size within 0.1÷0.5 mm; 2) conglomerates of weakly bonded finely dispersed (less than 0.1 mm in size) particles of zirconium dioxide. Scattered fine particles of ZrO$_2$, which do not belong to conglomerates, were assumed to be uniformly distributed in the volume of the cement matrix and were taken into account implicitly through the effective mechanical characteristics of the cement matrix. The materials of all components of model concrete were assumed to be isotropic and brittle. The values of their elastic and strength parameters are shown in table 1. The approximation of the ideal bonding of inclusions to the matrix was used.

| Table 1. Mechanical parameters of the components of model concrete (ZAC). |
|-----------------|-----------------|-----------------|
|                 | Cement matrix   | Large aggregates | Conglomerates |
| Young’s modulus, GPa | 55              | 172             | 27            |
| Poisson’s ratio  | 0.18            | 0.3             | 0.18          |
| Compressive strength, MPa | 170             | 2100            | 170           |
| Tensile strength, MPa | 75              | 830             | 75            |

We considered 2D samples of ZAC with linear dimensions of 2x3 mm and a volume fraction of aggregates from 10% to 50% (figure 1a-c). Samples of the cement matrix without reinforcing ZrO$_2$ aggregates, but containing “soft” inclusion (micropores with a size of 10 μm, figure 1d) were additionally investigated. The volume fraction of pores in the samples was assumed to be 6%. This corresponds to the estimates of cement stone microporosity in real high-strength concretes.

![Figure 1](image_url)

**Figure 1.** Examples of mesoscale concrete samples with different volume fraction of inclusions: 10 vol% ZrO$_2$ (a); 30 vol% ZrO$_2$ (b); 50 vol% ZrO$_2$ (c); 6 vol% pores (d). Blue areas indicate the cement matrix, purple areas are solid ZrO$_2$ aggregates, and green areas are conglomerates of weakly bonded finely dispersed particles of ZrO$_2$.

Within the framework of the applied discrete element model of dynamic mechanical behavior of brittle solids [9], a local fracture is modeled by breaking the bond between two discrete elements when fulfilling a specified dynamic fracture criterion. In the study, we used the dynamic formulation of the Drucker-Prager criterion proposed earlier by the authors [11,12]:
\( \sigma(t) = \sigma(t) = \sigma_{eq}(t)0.5(a+1) + \sigma_{\text{mean}}(t)1.5(a-1) \geq \sigma_{\text{dyn}}(t-t_0) \), \hspace{1cm} (1)

where \( \sigma_{\text{mean}} \) is mean stress, \( \sigma_{eq} \) is equivalent stress, \( a = \sigma_{\text{dyn}}(t)/\sigma_{\text{dyn}}(t-t_0) \) is the relation of uniaxial compressive \( \sigma_{\text{dyn}} = \sigma_{\text{dyn}}(t-t_0) \) and tensile \( \sigma_{\text{dyn}} = \sigma_{\text{dyn}}(t-t_0) \) dynamic strengths, \( t_0 \) is a point of time at which the static strength is achieved (the criterion (1) is fulfilled with the use of the static compressive \( \sigma_{\text{st}} \) and tensile \( \sigma_{\text{st}} \) strength instead of dynamic values), \( t \) is the current time.

The “reference” dependencies (master curves) that relate the dynamic strength parameters \( \sigma_{\text{dyn}} \) and \( \sigma_{t\text{dyn}} \) with the local fracture time \( T_{\text{fract}} \) must be specified to implement the criterion (1). During the numerical simulation, the fulfillment of the “static” formulation of the Drucker-Prager fracture criterion (1) with \( \sigma_{\text{st}} \) and \( \sigma_{t\text{st}} \) as parameters is analyzed at each time step for each pair of chemically bonded discrete elements. When the “static” criterion is fulfilled for a pair, the process of incubation (formation) of local fracture begins. At each subsequent integration step, the dynamic criterion (1) is analyzed for this pair using the master curves \( \sigma_{\text{dyn}}(T_{\text{fract}}) \) and \( \sigma_{t\text{dyn}}(T_{\text{fract}}) \) (assuming \( T_{\text{fract}} = t-t_0 \)). When the dynamic criterion (1) is satisfied, the local fracture is considered to have occurred.

The authors previously showed that although the dependencies \( \sigma_{\text{dyn}}(T_{\text{fract}}) \) and \( \sigma_{t\text{dyn}}(T_{\text{fract}}) \) are individual for each material, they can be approximated with adequate accuracy by single functions (common for many brittle materials) expressed in terms of normalized (dimensionless) parameters [9]. These functions were used in this study as master curves. When using such functions, it is necessary to take into account the spatial scale of the local fracture area. The basic reference functions [9] were built using the experimental data on the fracture of macroscopic samples. Following the principles of the structural-kinetic theory of strength [13-15], these functions should be scaled along the time axis \( \sigma_{\text{dyn}}(T_{\text{fract}}) \) and \( \sigma_{t\text{dyn}}(T_{\text{fract}}) \) to adequately estimate the local fracture time in a mesoscopic sample (time of bond breaking in a pair of discrete elements). Here \( S_f \) is a dimensionless coefficient. It is defined as the ratio of the fracture time scale of the considered area to the fracture time scale of standard macroscopic samples used to obtain basic reference functions. The relationship between the \( S_f \) value and the ratio of the spatial scales of fracture is a matter of discussion for composite materials. Therefore, three different \( S_f \) values were considered in the study: \( S_f = 0 \) (the approximation of “instantaneous” crack incubation, which is typically used in conventional mechanical behavior models), \( S_f = 10^{-3} \) (corresponds to the transition from the spatial scale \( 10^{-2} \) m of standard macroscopic samples to a scale \( 10^{-5} \) m of a discrete element in a mesoscopic model sample), and \( S_f = 1 \) (corresponds to the fracture time of standard macroscopic samples).

The uniaxial compression tests at a constant strain rate \( \dot{\varepsilon} \) were simulated. The values of the strain rate ranged from \( 1 \) s\(^{-1}\) to \( 10^3 \) s\(^{-1}\). The influence of the strain rate on the strength characteristics (dynamic strength and fracture time) of mesoscale samples was analyzed.

3. Results

3.1. Influence of reinforcing aggregates

The simulation results showed that strain rate dependence of the strength of the mesoscale samples has a pronounced nonlinear form. Figure 2a shows examples of such dependences for the samples with 30 vol\% ZrO\(_2\) at various values of \( S_f \). One can see that an increase in the sample strength with an increase in the strain rate can be described by a power function, and the value of fracture time scale coefficient \( S_f \) strongly determines the value of the exponent of this function.
Figure 2. Dependences of the normalized dynamic strength (a) and fracture time (b) on the strain rate at various $S_f$ values for mesoscopic concrete samples with a volume fraction of aggregates of 30%. Normalized dynamic strength hereinafter is defined as the ratio of the absolute value of dynamic strength to the value of strength under quasistatic loading (<$10^{-3}$ s$^{-1}$). Solid black curves show the analytical estimations of strength and fracture time for macroscopic concrete samples [9].

At the $S_f=1$ (macroscopic fracture time for the pairs of discrete elements), the strength of mesoscale concrete samples significantly exceeds the “reference” values for macroscopic samples (1÷10 cm in size). At the same time, for $S_f=10^{-3}$ (proportional scaling of the fracture time and the linear size of the fracture region, that is assumed in the framework of the classical concept of the structural-kinetic theory of strength) we can see a significant decrease in the dynamic strength of mesoscale samples in comparison with the “reference” values (solid black curve in figure 2a) for macroscale samples. The effect of an increase in strength is extremely small and almost does not differ from the limiting case of instantaneous fracture time ($S_f=0$). In addition to increasing the strength, the scale factor $S_f$ also affects the time of sample fracture (figure 2b). The fracture time curve for model samples at $S_f=1$ agrees with good accuracy with the analytical estimation for macroscale samples, however, the fracture time at $S_f=10^{-3}$ is 3÷5 times lower than the analytical macroscopic estimation.

The simulated samples have linear dimensions of the order of $10^{-3}$ m and contain a sufficient number of mesoscopic inclusions, i.e. they are representative volumes of material. Therefore, the value of dynamic strength at a given strain rate should be close to the corresponding value of the strength of typical macroscopic samples of 1÷10 cm in size. Figure 2a shows that this requirement is achieved neither by using the basic master curves ($S_f=1$) nor by functions proportionally scaled to mesoscopic spatial scale ($S_f=10^{-3}$). A special study showed that the requirement for the proximity of the dynamic strength of the mesoscale sample to “reference” (macroscopic) value is fulfilled when using $S_f\approx 10^{-1}$. This is a result of the change in the conditions and dynamics of the formation and growth of ensemble of microscale discontinuities in the regions of cement matrix constrained by reinforcing aggregates.

Thus, the scaling of the macroscopic master curves $\sigma_{c}^{\text{dyn}}(T_{\text{frac}})$ and $\tau_{t}^{\text{dyn}}(T_{\text{frac}})$ in proportion to the spatial scale of the fracture region is insufficient and may even be fundamentally incorrect when modeling the mesoscale samples with an explicit composite structure. Such scaling does not take into account the peculiarities of the formation of the system of discontinuities. These peculiarities are manifested when going down from a homogeneous macroscopic structure to a mesoscopic representative volume (different phases of the composite structure are clearly expressed on this scale).

Similar studies for other values of aggregate concentration showed that the difference in the values of the normalized dynamic strength and fracture time between samples with different volume fractions of reinforcing aggregates is not large, however, it increases monotonically with increasing strain rate. This is the result of an increase in the duration of the initial stage of discontinuities accumulation, as well as a significant complication and extension of the path of fracture cracks. The results obtained
lead to the conclusion that the key factor determining the rate of change of the local fracture time when changing not simply the spatial but the structural scale is the factor of the interface zones on which primary microcracks are predominantly localized.

3.2. Influence of cement matrix porosity

The simulation results showed that a change in the spatial scale accompanied by a qualitative change in the multiphase structure leads to a breaking of the linear relationship between the incubation time and the size of the fracture region. For a more complete understanding of the influence of the structural factor, we carried out a similar study for unreinforced samples consisting of one phase (cement matrix) with “soft” inclusions (rounded pores). Similar to ZrO₂ aggregates, the pores are an essential factor determining the fracture time and strength characteristics of concrete. However, unlike reinforcing aggregates, the pores decrease the strength of the sample [16,17].

Figure 3a shows the dependences of the normalized strength of porous cement stone samples on the strain rate at various values of the scaling coefficient $S_f$. As in the case of reinforcing inclusions, the heterogeneous structure of the porous samples determines a breaking of the linear relationship between the spatial and temporal scales of fracture.

![Figure 3. Dependences of the normalized dynamic strength (a) and fracture time (b) of mesoscopic cement matrix samples with micropores on the strain rate at various $S_f$ values. Solid black curves show analytical estimations of strength and fracture time for macroscopic cement samples.](image)

Generally speaking, the results indicate that the nature of the change in the relationship between the temporal and spatial scales of fracture in brittle multiphase materials does not depend on the type of inhomogeneities (reinforcing inclusions or weakening pores), which arise/disappear when the scale changes. It is determined, first of all, by the presence of inhomogeneities and their quantitative concentration (the number of structural elements per unit volume). Following from figure 2b and figure 3b, the fracture time of cement stone samples with micropores is higher than for all considered concentrations of reinforcing inclusions despite a much lower volume fraction of pores. In the case of a porous sample, there is a high concentration density of inhomogeneities (pores), which even with their relatively small volume fraction provides a more significant effect on the process of crack system formation in the sample and, consequently, on the value of the fracture time. Thus, the quantitative concentration of inclusions (and the characteristic distance between inclusions) is no less an important factor for dynamic fracture than their volume fraction.

4. Conclusions

One of the key problems of computer design and virtual testing of multiphase materials with a multiscale composite structure, which are anticipated to function under intense mechanical impacts, is
the specifying of the dynamic mechanical characteristics of structure components (phases) and interface zones at low structural scales. This problem is relevant, in particular, for brittle materials. The macroscopic nonlinear behavior of this class of materials is determined by incubation and development of an ensemble of discontinuities of various sizes. A promising approach to the theoretical description and study of such materials at various structural scales and in a wide range of loading rates is an approach based on the principles of the structural-kinetic theory of strength. The key material parameter in this approach is the incubation (formation) time of the discontinuity. The identification of the scale and structural dependence of the value of this material parameter is one of the principal directions in the development of this concept as applied to multiphase materials.

The results of the theoretical study showed that the conventional idea about the linear nature of the relationship between the spatial and temporal scale of fracture is not acceptable if a change in the spatial scale is accompanied by a change in the structural pattern (i.e. a qualitative change in the structure). A technique has been developed to estimate the magnitude of the spatio-temporal scaling coefficients for the dynamic mechanical characteristics of the material with the use of experimentally determined values on macroscopic samples. Applying adequate scaling coefficients for different components and interfaces allows correct modeling of the dynamic mechanical behavior of composites at “low” structural scales. We showed that the scaling factors can be different for different components/interfaces. The results lay the physical foundation of the concept of multiscale computer design, modeling of mechanical behavior, and predicting the dynamic characteristics of composites.

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