Development of a discrete element approach for numerical study of features of fracture of composites with multiscale internal structure

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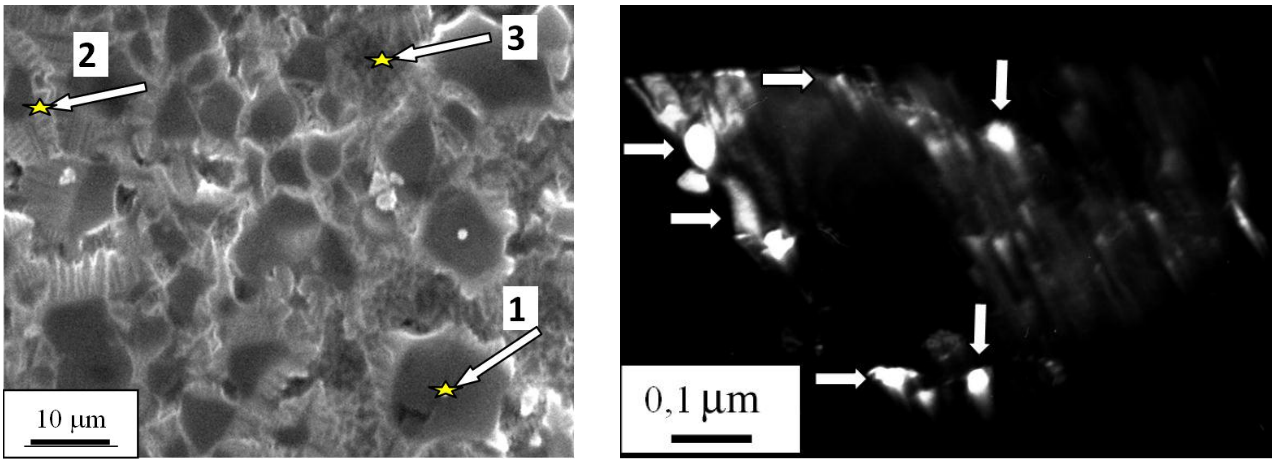
Abstract. The paper is devoted to development of the structural model of metal-ceramic composites within the framework of numerical discrete element method. The model takes into account main features of multiscale internal structure of composites such as content of reinforcing ceramic particles whose sizes are distributed within several structural scales, width and mechanical properties of transition zones at interphase boundaries and so on. Capabilities of the developed discrete element-based model are demonstrated by the example of numerical study of features of fracture of NiCr-based metal-ceramic alloy with TiC inclusions.

Introduction

An important direction in modern deformable solid mechanics is study and structural design of advanced tool materials for the purpose of improvement their operating characteristics. This problem is especially topical for metal-ceramic composites (MCC) which are used as materials for units (for example, cutting plates) working under conditions of intensive dynamic loading [1-3].

This class of materials is prepared by powder metallurgy methods, in particular, by sintering of powder mixtures of ceramic (for example, carbide) and metallic particles. One way to improve the physical and mechanical properties of the MCC is purposeful formation of multiscale phase structures in the surface layers of samples. A promising way to modify the surface layers of the MCC is a pulsed electron-beam radiation treatment.



a b

Fig.1. Microstructure of surface layer of metal-ceramic composite TiC-(Ni-Cr-Al) after pulsed electron-beam radiation treatment (a) and dark-field image of NiCr binder of modified surface layer in reflex [022]TiC (b). Arrows in (a) shows periphery of the particles of titanium carbide (1), transition zone from the carbide particles to the metallic binder (2) and metallic binder (3) containing submicron-scale TiC particles (small black points). Arrows in (b) shows TiC nanoparticles.

As previously shown by the authors by the example of metal-ceramic alloy TiC-(Ni-Cr), a multiscale internal structure is formed in a modified surface layers (Fig. 1) [4]. Main elements of this structure are: mesoparticles of refractory carbide, metal binder and interphase boundaries "particle-binder" (on the mesoscopic scale); secondary submicron-scale TiC particles distributed in the inter-particle space of metal binder (on the submicroscopic scale); secondary carbide nanoparticles aggregated at the boundaries of crystallization cells in the metal binder (on the nanoscopic scale).

These elements of the hierarchy of structural scale have non-additive effect on the integral characteristics of the alloy. Therefore understanding of contributions of structural constituents of different scales to mechanical response (including fracture development) of MC composites is a topical problem. This problem can be efficiently solved with help of computer modeling using particle-based methods. The present paper is devoted to development of formalism of the representative of particle-based discrete element approach (namely, of movable cellular automaton method [5,6]) to study features of fracture of MCC by the example of NiCr-based MC composite with TiC inclusions.

Mathematical model of metal-ceramic composite

Development of the formalism of discrete element method (DEM) to modeling MCC includes both development of structural model of metal-ceramic alloys and formulation of discrete element interaction forces to correctly simulate elastic-plastic deformation and fracture of constituents of composite.

To solve this problem the DE-based two-dimensional structural model of metal-ceramic alloy as a multiscale composite was built [4]. The model directly takes into account features of the geometry of reinforcing inclusions and their size distribution in a wide range of scales, as well as physical and mechanical properties of interphase boundaries (interface regions). In the framework of the model NiCr-based MCC is considered as a plastic matrix (binder) with integrated brittle high-strength TiC inclusions of mesoscopic scale size (1-10 μm). Each of constituents is modeled by ensemble of movable cellular automata (discrete elements) with appropriate rheological parameters. The size of a cellular automaton *d* is an assigned parameter of the model. In the considered model it was chosen taking into account the requirement that the value of *d* is few times greater than both the characteristic size of grains of the binder and typical size of mesoscopic TiC inclusions. Note that in this case the models of elastic-plastic isotropic media can be correctly applied to describe the deformation of discrete element with characteristic size *d*. The maximum value of the dimensional model parameter *d* determines level of detail of the description of TiC particle shape. The above defines an "optimum" of range of definition of the value of *d* for considered metal-ceramic composite as amounting to 0.1-0.3 μm.

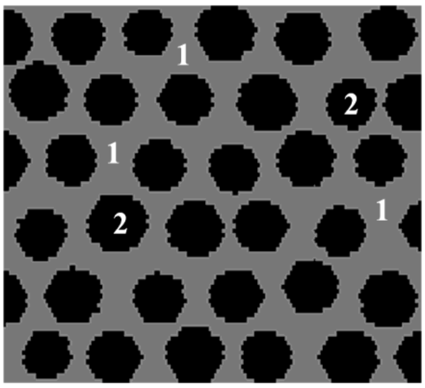


Fig.2. Structural model of metal-ceramic alloy. Main constituents of the structure are: nickel-chromium plastic binder (1) and high-strength brittle TiC mesoparticles (2).

As an example, Fig. 2 shows the structure of a model metal-ceramic composite with TiC particles have a shape close to spherical and the average size D_{TiC}=3 μm (the amplitude of the deviation from the mean value of the particles size in this example does not exceed $0.1 \cdot D_{TiC}$). The size of movable cellular automaton in this case is *d*=0,3 μm.

As follows from the data of electron microscopy, electron-beam modification of the surface layer of the composite leads to partial dissolution of TiC mesoparticles in the binder (and smoothing of their form) and precipitation of TiC particles of submicron TiC (0.2-0.3 μm) and nanoscopic (60-75 μm) scales from supersaturated solid solution (Fig. 1). To account for these structural features the mesoscopic structural model of modified surface layers of metal-ceramic alloy was developed. The structure of the modified composite is built on the basis of the structure of the initial composite through the "removal" fragments of TiC (automata with properties of TiC) from the most remote parts of the surface TiC mesoparticles (including their angular regions) and distribution of these fragments in the metallic binder near the corresponding mesoparticle. The volume fraction of "dissolved and precipitated" so the material is a model parameter and corresponds to the content of disperse TiC particles in the modified surface layer of real composite. Since the characteristic size of the secondary particles of submicron and nanoscopic scales differ by 3-5 times, ways to address their content in the binder are also different (Fig. 3):

1. "Submicron" secondary particle TiC is modeled explicitly by a single movable cellular automaton or a conglomerate of several elements [4].
2. The content of nanoscale (60-75 nm) of secondary particles is taken into account implicitly through a change in the response function (i.e., rheology) of movable cellular automata modeling binder. Note that experimental determination of changes in the rheological characteristics of the binder material in a consequence of precipitation of reinforcing nanoparticles is a difficult task. Therefore a phase mixture model could be used as a first approximation for the evaluation of parameters of the response function of cellular automata modeling volumes of binder containing nanoparticles. Within this model it is assumed that the presence of nanoparticles leads to enhancing integral hardening of the material and reduce the ultimate strain value. Magnitude of hardening and strain characteristics are model parameters associated with the local value of the volume content of nanoparticles.

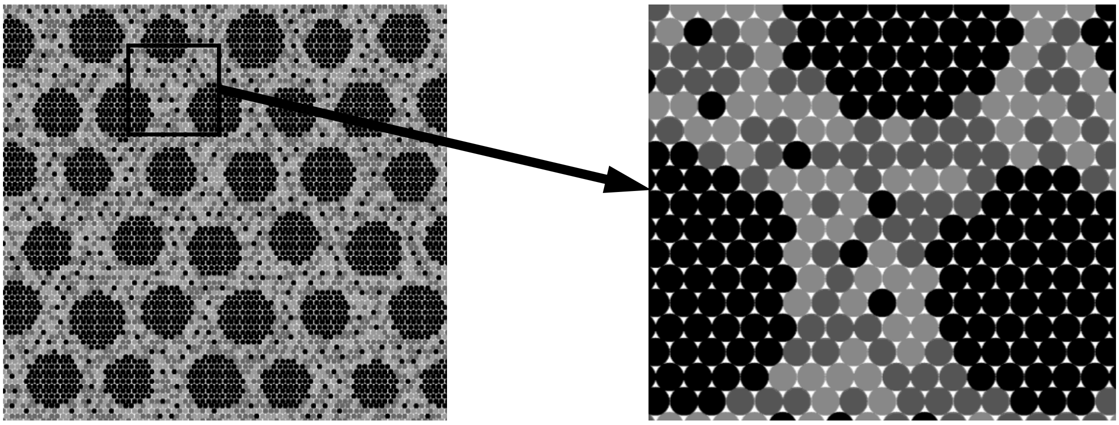


Fig.3. Structural model of modified surface layer of metal-ceramic alloy. Small black inclusions are precipitated (secondary) "submicron" particles TiC мелкие включения черного цвета – вторичные частицы TiC субмикронного масштаба, darker areas of binder model material (NiCr) containing nanoparticles of TiC.

An important part of the developed model of metal-ceramic composite is the account of the transition layer at the interface between the reinforcing particles and the binder. In particular, electron-beam modification of the surface layer with certain parameters of radiation can lead to a significant increase in the width of the transition layers at particle-binder interphase boundaries. Depending on the level of detail of the model there are two ways to account physico-mechanical and spatial (including width) characteristics of the transition layer:

1. The model of a "narrow" zone in which the width of the interface is assumed much smaller than the size of movable cellular automaton (Fig. 2). The defining properties of such a model of the interface are its strength characteristics. Note that this approximation does not account for features

of the rheology of the transition layer and can be used effectively in the case where the width of this layer does not exceed the assigned size of movable cellular automaton *d*.

2. The model of a "wide" interface, whose width is comparable to or greater than the size of the movable cellular automaton (Fig. 4). In this approximation, the interface is regarded as an area of variable composition and modeled by several layers of cellular automata, physical and mechanical characteristics of which vary in a given law. Relations between the change in the content of chemical elements (Ti, Ni, Cr et al.) with distance from the particle surface and the corresponding change in the rheological characteristics of cellular automata are determined on the basis of experimental data. This approach can be efficiently used in numerical models of composites in the case of assigned size of a cellular automaton *d* is not greater than the width of the transition zone.

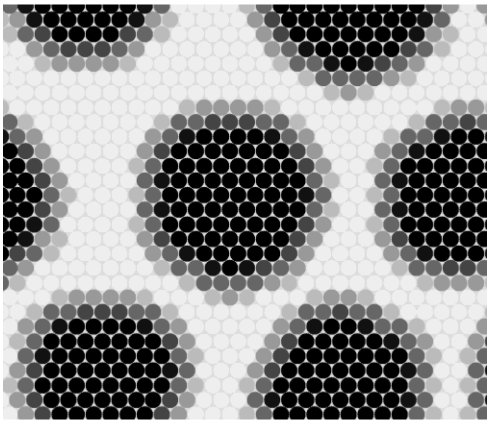


Fig.4. The internal structure of a model metal-ceramic composite with "wide" transition zone (~0.8 μm in the present example) from TiC particles (shown in black) to the NiCr binder (shown in light gray). Shades of gray color of varying intensity mark areas of the transition zone with appropriate content of Ti.

The main problem when using an explicit way of modeling the transition zone of the particle-binder interface is the determination of rheological parameters and strength of areas (layers) of this zone, located at different distances from the particle surface. Experimental determination of these parameters is extremely difficult problem. Therefore, a phase mixture model can be used as a first approximation with the assumption that the transition region has a structure similar to a solid solution of Ti (and C) in the NiCr matrix with decreasing concentrations of Ti and C with increasing distance from the surface of the particles to the binder.

In this model the rheological characteristics and strength of the regions (layers) of the transition zone are defined by linear interpolation of corresponding values for the components (TiC and NiCr), that is proportional to the local volume concentration of TiC. This approximation was used in the calculations carried out.

The components of the MCC have very different rheological characteristics (in case of considered composite these are elastic-brittle high-strength TiC inclusions and elastic-plastic NiCr binder).

For correct modeling of deformation and fracture of such complex systems the mathematical formalism of constructing many-particle interaction forces for cellular automata (discrete elements) with different rheological characteristics was developed [5,6]. Force of element interaction is written as a superposition of pair-wise component and volume-dependent component, connected with influence of surrounding discrete elements. A fundamental advantage of developed approach to building discrete element interaction is concerned with capability to realize various rheological models of material behavior within various realizations of discrete element method. In particular, an incremental theory of plasticity of isotropic medium with von Mises plasticity criterion was implemented within the framework of DEM to model deformation of metallic binder on the mesoscopic scale [5,6]. Radial return algorithm of Wilkins [7] was adopted for this purpose. Elastic constants and the diagram of uniaxial tension was used as input parameters of the model of plasticity for the NiCr binder.

The developed concept of many-body interaction of discrete elements makes it possible to use multiparametric fracture criteria (Drucker-Prager, Mohr-Coulomb etc.) as criteria of interelement bond breakage. In particular, in the described model Drucker-Prager fracture criterion was used to describe the fracture of metallic binder and carbide particles. The following notation of this criterion was used:

$$\sigma_{\text{int}}^{ij} 0.5(a+1) + \sigma_{mean}^{ij} 1.5(a-1) > \sigma_c , \qquad (1)$$

where σ_c is assigned threshold value for considered pair of cellular automata *i* and *j* (value characterizing strength of chemical bond under uniaxial compression), *a* is a ratio of bond compressive strength to tensile strength, σ_{int}^{ij} and σ_{mean}^{ij} are stress intensity and mean stress calculated at the contact point of the pair *i*-*j*. A detailed description of the method of calculation of these variables is given in the paper [6].

Computational study of influence of interphase boundaries on fracture and mechanical properties of MCCs

The developed particle-based model of the MCC is used to theoretical study of features of fracture of the composite on the basis of titanium carbide TiC with a metallic binder of nickel-chromium alloy. Note that a key element of the structure that determines the strength and deformation properties of the composite as a heterogeneous multiphase system are the interfaces (interphase boundaries) of the metal matrix and the reinforcing TiC particles. In the present work a theoretical study of the influence of this structural factor on the response (including fracture) of metal-ceramic alloy TiC-(NiCr) under dynamic loading was carried out.

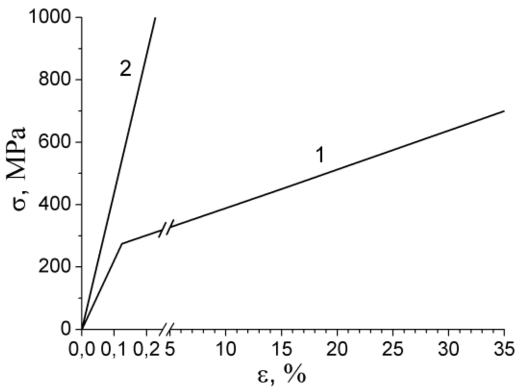


Fig.5. The response functions of movable cellular automata modeling (NiCr)-alloy (1) and titanium carbide TiC (2).

To model the elastic-plastic metallic binder the parameters of mechanical response of movable cellular automaton conforming to the mechanical properties of nickel-chromium alloy were chosen. The response function of automaton modeling NiCr was considered as stress-strain diagram with linear hardening (curve 1 in Fig. 5). This diagram is an approximation of the experimental diagram of uniaxial compression of macroscopic samples of the alloy. Mechanical properties of automata that simulate high-strength brittle inclusions, meet the real properties of TiC particles in the ceramic phase (polycrystalline particles, curve 2 in Fig. 5). Note that the function of mechanical response of movable cellular automaton is an analog of a unified deformation diagram used in the mechanics of deformable solids to describe the elastic-plastic behavior of materials [6].

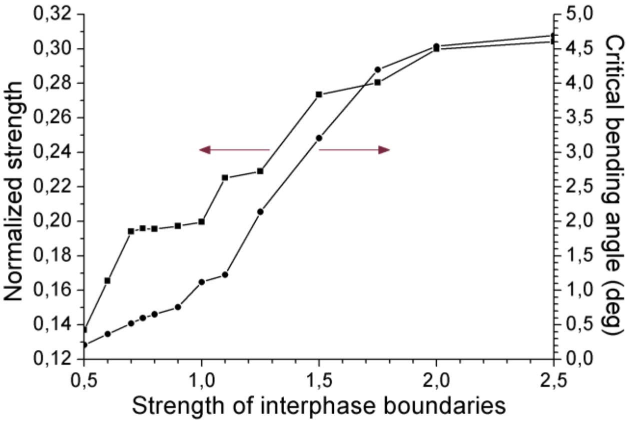
It is well known that the service characteristics of metal-ceramic alloy (as well as of other composite materials) is largely provided by the quality of adhesion of the binder to the reinforcing inclusions. Therefore, in the ongoing study the influence of strength of particle-binder interfaces on the integral parameters of the mechanical response of the composite (such as strength, ultimate strain and fracture energy) and pattern of fracture under dynamic impact was analyzed. A numerical model of an alloy with "sharp" (narrow) interphase boundaries (Fig. 2) was used. A two-parameter criterion of Drucker-Prager (1) was applied as a criterion of interelement bond breakage (fracture criterion). The following parameters of this criterion for constituents of the composite were chosen:

1. (NiCr)-alloy: σ_t^{NiCr}=700 MPa, $a_{NiCr} = \sigma_c^{NiCr} / \sigma_t^{NiCr}$=3.

2. TiC: σ_c^{TiC}=10000 MPa, $a_{TiC} = \sigma_c^{TiC} / \sigma_t^{TiC}$=5 (estimate of the value of a_{TiC} made under the assumption about the absence of significant defects in TiC particles).

3. Interphase boundary: the value σ_t^{bound} was considered as a variable parameter and varied within the limits between $0.5\sigma_t^{NiCr}$ and $2.5\sigma_t^{NiCr}$. The parameter a_{bound} in the criterion (1) was assumed to

be 3 in all calculations.
Three-point bending test on model samples of metal-ceramic composite TiC-(NiCr) with dimensions of 24×130 μm was simulated. Dynamic loading by cylindrical mandrel with constant velocity V_{load}=0,4 m/s was applied.
The simulation results showed that the change in interface strength (σ_t^{bound}) leads to a directional change in the integral characteristics of the composite response of 2-10 times. In particular, increasing the strength of the interphase boundaries leads to a twofold increase in the strength of the composite, as well as the increasing of the value of the limit strain (critical value of bending angle in considered test) and fracture energy by an order of magnitude (Fig. 6).



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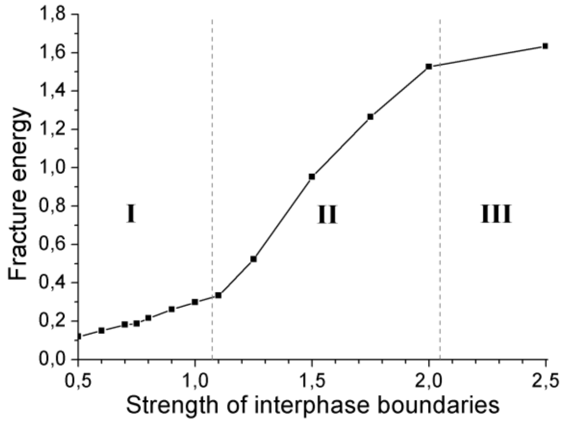

b

Fig.6. Dependencies of normalized strength of model metal-ceramic composite, its critical strain (value of bending angle at the start of main crack propagation) (a) and fracture energy (b) on interphase boundary strength (interface strength is expressed in normalized units $\sigma_t^{bound}/\sigma_t^{NiCr}$). Fracture energy was defined as an area under the loading diagram expressed in the units "normalized stress – bending angle".

The analysis of simulation results showed that the change of integral parameters of the composite response with increase of strength of interphase boundaries (σ_t^{bound}) has a pronounced non-linear character (Fig. 6) and is associated with a change in the nature of fracture. At low values of interface strength σ_t^{bound} (smaller than the strength of metallic binder σ_t^{NiCr}) already in the early stages of loading (at small applied deformations) TiC particle are detached from the binder on the extended sites of phase boundaries, which are under the condition of tensile stress (top row in Fig. 7). With increasing the applied strain these sites of separation of composite constituents are consequently connected by cracks passing through the binder, into a single main crack. At the same time, at high values σ_t^{bound}, approaching the strength of reinforcing particles themselves, the cracks are formed and distributed in the matrix, bypassing interphase boundaries, while interface zones remain virtually intact (bottom row in Fig. 7). In the "intermediate" range of interface strength (σ_t^{bound} is equal to or somewhat greater than the value of strength of the binder) character of the composite failure changes from "interfacial" type to a "matrix" type. It is clear that initiation of cracks in the plastic binder takes place at large applied deformations, and crack development is rather slow. As a consequence fracture energy of composites with high-strength interface boundaries increases by an order of magnitude (Fig. 6b). Thus, the strength of interfaces between reinforcing inclusions and plastic binder is a critical factor, which determinings a number of service characteristics of metal-ceramic composites, such as strength, critical strain, crack growth resistance and others.

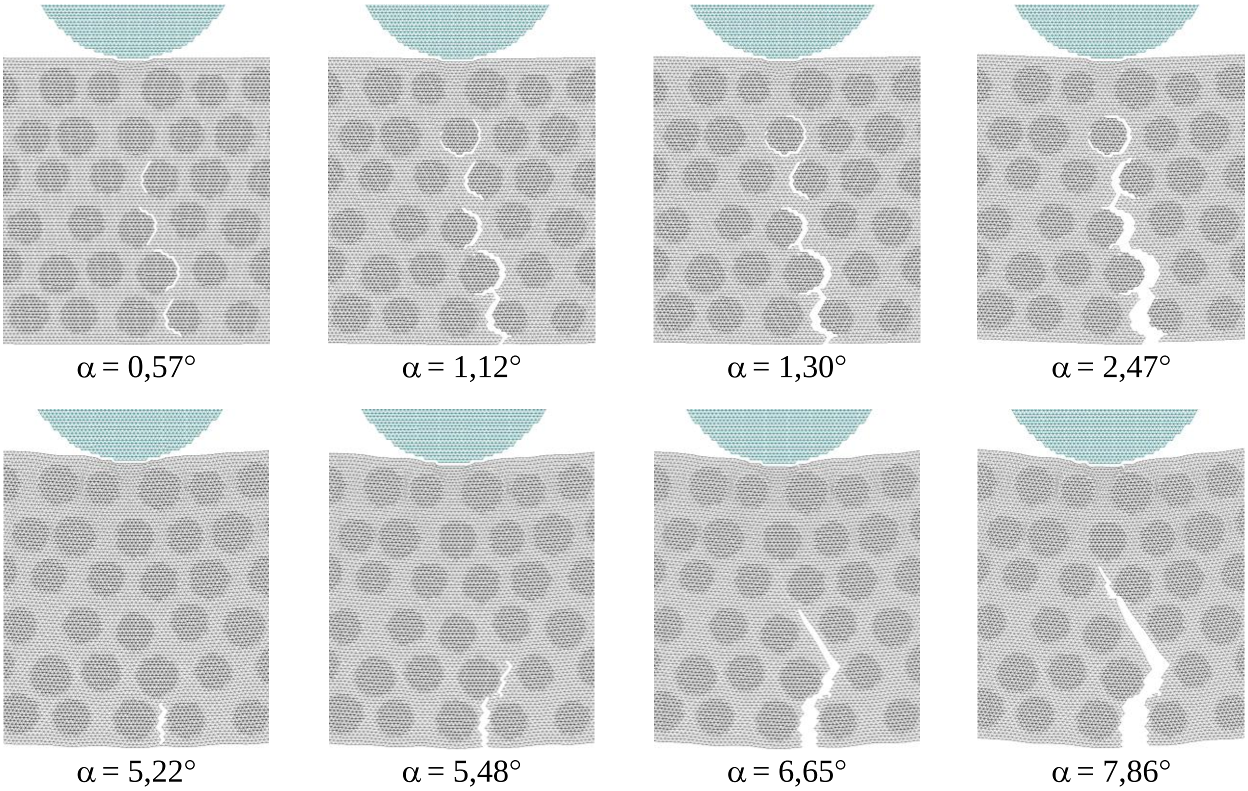

Fig.7. Dynamics of fracture of metal-ceramic composite specimens characterized by different values of the strength of interface boundaries σ_t^{bound}: $0{,}7\,\sigma_t^{NiCr}$ (top row); $2{,}5\,\sigma_t^{NiCr}$ (bottom row). Hereinafter α is bending angle.

In addition to the interface strength, an important characteristic of interphase boundaries defining their deformation ability and effective strength is the width of the zone of variable composition of chemical elements (transition zone). Simulation results showed that the increase in the width of the transition zone (Fig. 4) is accompanied by a decrease in the value of stress gradient at the interfaces due to the reduction of the gradient of mechanical properties.

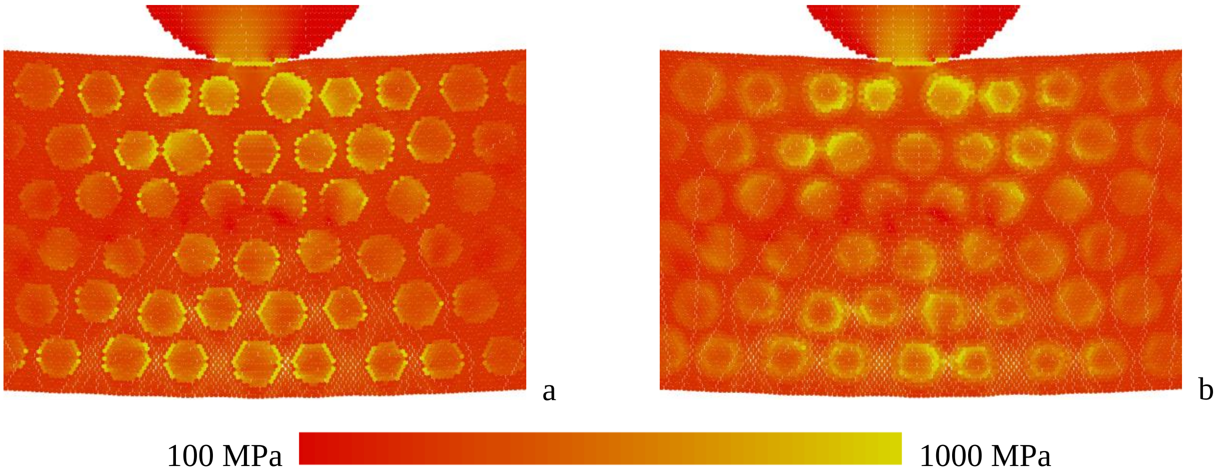

Fig.8. Stress intensity distribution in the central part of MCC samples with “narrow” (a) and “wide” (b) interphase boundaries (α = 3,5°). Three-point bending test.

This leads to a sharp increase in the strength and deformation characteristics of the composite, as well as the fracture energy. The values of these parameters approaches to the maximum corresponding to the "original" (before surface treatment) composites with narrow high-strength interphase boundaries (regions $\sigma_t^{bound} > \sigma_t^{NiCr}$ in Fig. 6). This change in the service characteristics of metal-ceramic alloy is concerned with two-threefold decrease in the value of stress gradient on the "fuzzy" (wide) interphase boundaries (Fig. 8) due to the reduction of the gradient of mechanical properties. The consequence is the increase of deformation and strength characteristics of the composite and the change in the type of fracture from "interfacial" (inherent in composites with low-strength narrow interfaces) to cracking in the binder. Also note that the appearance of relatively wide transition zones at the interfaces (Fig. 4) leads to an increase in the slope of the hardening curve by up to 30-40%. This is due to a decrease in the volume fraction of "unmodified" plastic (NiCr)-alloy and corresponding increase in fraction of stronger and less ductile wide transition regions at the interphase boundaries.

Summary

The mathematical formalism of discrete element method (DEM) for numerical simulation of deformation and fracture of composite materials with multiscale internal structure, including metal-ceramic composites (MCC) with refractory reinforcing particles and metallic binder, is developed. To adequately describe these complex systems fundamentals of structural model of metal-ceramic composites are formulated. They take into account a multiscale structure of the material and the presence of extended transition zones at the interphase boundaries, characterized by a certain gradient of the physical and mechanical properties. The developed structural model of metal-ceramic composites and corresponding expressions for many-body interaction of discrete element modeling metallic binder and brittle ceramic particles are implemented within the framework of a representative of the DEM, namely, the computational method of movable cellular automata (MCA). It is necessary to note the generality of the proposed model of MCC, which features make it possible to study patterns of deformation and fracture of composite materials of different nature within a single formalism.

With the use of the formalism the influence of some key structural parameters on the mechanical properties of the metal-ceramic alloy TiC-(Ni-Cr) under intense dynamic loads was studied. In particular, it is shown that the formation of extended (wide) transition zones at the interphase boundaries leads to a considerable increase in the strength and deformation characteristics of the composite, as well as an increase in the fracture energy by an order of magnitude. The simulation results indicate the possibility of managing a set of service characteristics of metal-ceramic composites (hardness, strength, deformation capacity, fracture energy etc.) by means of changing the width of the interphase boundaries and the profile of the transition zones.

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