Development of a structural and rheological model for investigation of peculiarities of deformation and fracture of metal-ceramic composites with multimodal internal structure

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Abstract

Paper is devoted to development of structural and rheological model for investigation of peculiarities of deformation and fracture of metal-ceramic composites in the framework of movable cellular automaton method (one of the representatives of discrete element methods in computational mechanics). Developed model takes into account main features of internal structure of metal-ceramic composites, such as wide size distribution of reinforcing ceramic inclusions, presence of wide transition zones between inclusions and metallic binder, etc. Using this model influence of width of interphase boundaries on the strength, the value of the ultimate strain and fracture energy of metal-ceramic composites was theoretically investigated. It is shown that the formation in the material of relatively wide interphase boundaries, characterized by a smooth change of the mechanical properties during the transition from the surface of ceramic inclusions into the volume of the binder, can significantly improve the mechanical properties (strength and fracture energy) of the metal-ceramic composite. This effect is connected with a significant decrease in stress gradient on the wide interphase boundaries.

Keywords: Metal-ceramic composites; interphase boundaries; computer-aided simulation; strength; fracture energy.

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1. Introduction

Metal-ceramics alloys are representatives of particle strengthened composite materials. They are characterized by high values of mechanical and operational characteristics such as strength, hardness, durability, crack resistance, thermal stability, etc. This makes metal-ceramic composites very attractive for a wide application in various industrial fields as materials used in extreme conditions (Chawla and Chawla, 2006). In particular, such materials are widely used in the manufacture of metalworking tools. So, an important direction in modern deformable solid mechanics is study and structural design of metal-ceramic composites for the purpose of improvement their operating characteristics. This class of materials is prepared by powder metallurgy methods, in particular, by sintering of powder mixtures of ceramic and metallic particles. Mechanical and physical properties of sintered metal-ceramic composites, in addition to the phase composition, are determined by a number of structural factors. Among them there are volume content, dispersion, geometry and defective structure of reinforcing particles of refractory compounds, structural-phase state of the metallic binder, the quality of the adhesion between the binder and inclusions (Ayyar and Chawla, 2006; Kulkov, 2005). A promising way to improve mechanical characteristics of metal-ceramic composites is a purposeful formation of high-strength multiscale phase structures in the surface layers by pulsed electron-beam irradiation (Psakhie, Shilko et al., 2013; Psakhie, Ovcharenko et al., 2013). For example, such surface treatment of sintered alloy 50 vol.% TiC-50 vol.% NiCr leads to a considerable increase in the mechanical and service characteristics of the surface layer. Results of experimental investigations showed that increasing of the operational characteristics of the modified composite is associated with the formation in the surface layers of the multimodal (multiscale) internal structure. One of its main elements are relatively wide transition zones at the titanium carbide-metallic binder interfaces. These zones are characterized by concentration gradient of chemical elements (Ti, C, Ni and Cr) and as a consequence, the gradient of mechanical properties with increasing distance from the surface of the inclusion.

Interfaces between the reinforcing particles and metal binder are one of the main elements of the internal structure of metal-ceramic composites. Influence of interphase boundaries on the mechanical properties of composite materials are discussed in a large number of papers (Lurie et al., 2006; Singh et al., 2007; Tran et al., 2010). Thus, the interphase boundaries in the metal-ceramic composites are important structural elements having their own set of dimensional, structural and mechanical characteristics. Therefore, the formation of wide interphase boundaries in the surface layers of metal-ceramic composites after of electron-beam treatment should be one of the main reasons for increasing of operational characteristics of the material. Experimental study of the effect of this factor on the properties of metal-ceramic composites is quite difficult problem. So, it can be efficiently solved with help of computer modeling using particle-based methods. The present paper is devoted to development of a structural and rheological model of metal-ceramic composites in the framework of movable cellular automaton method (Psakhie, Horie et al., 2011; Psakhie, Shilko et al., 2011; Psakhie, Shilko et al., 2013) for investigation of influence of the width of interphase boundaries on peculiarities of deformation and fracture of metal-ceramic composites.

2. Structural and rheological model of metal-ceramic composite

To achieve the objectives of the paper a two-dimensional structural and rheological model of the composite material was developed in the framework of movable cellular automaton method. In this model NiCr-based metal-ceramic composite is considered as a plastic binder with integrated brittle high-strength spherical TiC inclusions of mesoscopic scale size (1-10 μm). Each of constituents is modeled by ensemble of movable cellular automata with appropriate rheological parameters. Volume content of ceramic inclusions was equal to 50 vol.%. As an example, fig. 1a shows the structure of a model metal-ceramic composite with TiC particles have a shape close to spherical and the average size 3 microns. The components of the metal-ceramic composites 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 with different rheological characteristics was developed (Psakhie, Horie et al., 2011; Psakhie, Shilko et al., 2011; Psakhie, Shilko et al., 2013). 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 movable cellular automaton method to model deformation of metallic binder on the mesoscopic scale (Psakhie, Horie et al., 2011; Psakhie, Shilko et al., 2011; Psakhie, Shilko et al., 2013). Radial return algorithm of Wilkins was adopted for this purpose. Capabilities of the developed model makes it possible to describe the mechanical response (including fracture) of elastic-brittle and elastic-plastic isotropic media within approximations of plane stress and plane strain states (in the following calculations the plane stress approximation is used). Elastic constants of the material and the diagram of uniaxial loading are used as input parameters for the model of interaction of cellular automata. These parameters determine mechanical response function of movable cellular automaton. 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. 1b). 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. 1b).

Fig. 1. Structural model of metal-ceramic composite (a) and the response functions of movable cellular automata (b). Main constituents of the structure are: nickel-chromium plastic binder (1) and high-strength brittle titanium carbide inclusions (2).

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 two-parameter Drucker-Prager fracture criterion was used to describe the fracture of metallic binder and carbide particles (Psakhie, Horie et al., 2011; Psakhie, Shilko et al., 2011; Psakhie, Shilko et al., 2013). Thus, in this work the strength characteristics of the composite material are determined by the tensile and compressive strength of its components.

An important part of the developed model of metal-ceramic composite is the account of the wide transition layer at the interface between the reinforcing particles and the binder. In the paper it was taken into account using a mesoscopic model of “wide” transition zone whose width is comparable to or exceeds the size of the movable cellular automata (Psakhie, Ovcharenko et al., 2013). In this approximation, particle/binder interface is regarded as an area (zone) in which there is a systematic change of the volume concentration of the main components of the composite (TiC and NiCr) and, as a consequence, of the rheological properties with a distance from the ceramic particle surface into the volume of the binder. So interphase boundary is modeled by several layers of cellular automata. This approach can be efficiently used in numerical models of composites in the case of assigned size of a cellular automaton is not greater than the width of the transition zone. Relations between the change in the content of chemical elements (TiC and NiCr) 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. In the paper a special algorithm of creation of wide interface boundaries was developed on the basis of analysis of experimental
data. This algorithm uses information about a change in characteristic particle size during composite treatment and resulting profile of distribution of chemical elements in formed transition layer. So, developed approach allows to form in the model composite transition regions around carbide inclusions with a given concentration gradient of chemical elements and, consequently, given gradient of mechanical properties. The main problem in this model is the determination of rheological and strength parameters of 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 with the assumption that the transition zone has a structure similar to the solid solution of titanium and carbon in the metallic binder. Their content in the binder decreases with increasing distance from the particle surface. In this model the rheological characteristics and strength of the layers of the transition zone that are at different distance from the inclusions surface are defined by linear interpolation of corresponding values for TiC and NiCr (that is proportional to the local volume concentration of TiC).

It should be noted that the investigation of the peculiarities of the mechanical response of the modified surface layers of metal-ceramic composite was performed using a so-called multiscale approach. In the framework of this approach the elements of the composite internal structure of the mesoscopic scale (binder, primary particles TiC and wide interphase boundaries) are taken into account explicitly. Account of structural elements of lower scales (in particular, the presence of secondary titanium carbide nanoparticles in the interphase boundaries) is carried out by considering of structural models of a lower scales (in this case the submicron scale) with explicit account of concentrations, sizes and spatial distribution of nanoscale elements. On the base of analysis of simulation results of mechanical tests of submicron size samples their integral mechanical (including rheological) properties are determined. In the subsequent they are used as input data for cellular automata for modeling of composite response at the mesoscopic scale. In this paper, this approach was used for determining dependences of the rheological properties of the transition zones on the volume content of titanium carbide in nichrome binder.

3. Results of computer-aided simulation

Three-point bending test on model samples of metal-ceramic composite was simulated for investigation of influence of interphase boundaries width on mechanical characteristics of modified surface layers (fig. 2). Above described algorithm of explicit account of wide interphase boundaries, characterized by smooth gradient of changing of mechanical characteristics during the transition from the ceramic inclusion surface into the volume of the binder was used. Note that the TiC inclusion in real metal-ceramic composite can contain damages and microcracks. To eliminate the influence of this factor on the results of simulation in the paper it is assumed that the TiC particles in the model material have a "monolithic" structure and do not contain defects of meaningful scale. In the simulated tests loading by cylindrical mandrel (diameter of mandrel was equal to 20 microns) with a constant velocity was applied to the model sample with dimensions of 24×130 microns (fig. 2). As noted in the introduction, the products of ceramic-metal composites are often operated in complex extreme conditions. Therefore dynamic mode of loading with the loading speed of 1 mps was considered in the paper. The maximum value of bending resistance force (strength), corresponding value of mandrel displacement (critical bending angle) and fracture energy were analyzed.

Fig. 2. Scheme of the simulation of three-point bending test of the model composite sample.

The simulation results showed that increase of the width of the interphase boundaries leads to an increase in the strength of the composite, as well as the increasing of the value of the ultimate strain (critical value of bending angle
in considered test) and fracture energy (fig. 3). It is necessary to note, that values of strength of the composite in fig. 3a are shown in dimensionless form obtained by normalizing of the corresponding values of composite strength on the value of the tensile strength of the nichrome binder. Fracture energy was calculated as an area under the loading diagram expressed in the units “normalized stress – bending angle” (here “normalized stress” also has dimensionless form obtained by normalizing of the corresponding values of stress on the value of the tensile strength of the nichrome binder). As follows from the analysis of presented in fig. 3 dependences the main effect of increasing of the width of the interphase boundaries up to 1.6 microns is manifested in the increase in the critical strain of the material (2 times), and hence the fracture energy.

Fig. 3. 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 width (interface strength is expressed in normalized dimensionless units).

Fracture energy was defined as an area under the loading diagram expressed in the units “normalized stress – bending angle”.

Analysis of the results of computer-aided simulation showed that the increase in strength and value of ultimate strain of the composite material with the increasing of width of the interphase boundaries is due to the significant expansion of the region of the stress reducing from the high values in the reinforcing particles (which are stress concentrators in the composite) to significantly lower values in the plastic binder. Von Mises stress distributions for sample which are characterized by different width of interphase boundaries are shown in the fig. 4. It can be seen, that formation around the reinforcing particles of wide transition zones, which are characterized by a smooth change of the mechanical characteristics with the distance from the surface of the ceramic inclusion into the volume of the binder, leads to a "smearing" of the stress field and, consequently, to reducing stress gradient at the interfaces. This means that formation in surface layers of metal-ceramic composites of wide interphase boundaries between reinforcing particles and metallic binder interfaces provides a relatively low level of stress in the transition zones. This leads to increase of deformation ability and strength of the modified surface layers. Formation of such wide interphase boundaries may be perfume on the base of electron-beam irradiation of the surface of the composite.

Fig. 4. Von Mises stress distributions in the central part of model metal-ceramic composite samples with "narrow" (0.1 microns) (a) and “wide” (1.6 microns) (b) interphase boundaries (value of bending angle is 3.5°).
4. Conclusions

One of the most important structural factors that determine operational characteristics of metal-ceramic composites are interfaces between high-strength reinforcing inclusions and plastic metallic binder. Main reason of this effect is significant difference in elastic and rheological characteristics of the components of such composites. This leads to local stress concentration at the interfaces in the process of deformation of material. Therefore, account of physical and mechanical properties of interphase boundaries between reinforcing inclusions and the binder is an important problem in development of composite materials.

In this paper the influence of the width of interphase boundaries between reinforcing inclusions and metallic binder on mechanical properties of metal-ceramic composites under dynamic loading was theoretically investigated on the basis of computer-aided simulation by movable cellular automaton method. For this structural and rheological model of the composite, taking into account the main features of its mesoscopic structure was developed. The simulation results showed that the presence of wide transition zones at the interfaces of the ceramic inclusions and the metallic binder increases the strength, ultimate strain and fracture energy of the composite. This effect is associated with a significant decrease in stress gradient on the wide interphase boundaries characterized by a smooth change of the mechanical properties of the material in the transition zones.

It is necessary to note, that one of the most promising ways to improve the operational characteristics of metal-ceramic composites is the modification of their surface layers by electron-beam irradiation. As evidenced by the experimental data, such treatment leads to the formation in the surface layers of the composite of multiscale internal structure, which contains wide interphase boundaries. Operational characteristics of the obtained composites (strength, hardness, wear resistance, etc.) greatly depend on the parameters of the treatment (pulse duration, energy density of the electron beam, etc.). This effect is connected with peculiarities of the internal structure and, consequently, the mechanical properties of formed interphase boundaries during electron-beam irradiation. Thus, formation of surface layers characterized by a smooth changing of mechanical properties during the transition from the surface of the ceramic inclusions into volume of the metallic binder leads to increase in strength and deformation characteristics of the material.

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