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Study of the Influence of Morphology and Strength of Interphase Boundaries on the Integral Mechanical Properties of NiCr-TiC Composite

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Abstract. Sintered metal-ceramic materials are characterized by high mechanical and tribological properties. A key element of the internal structure of the metal-ceramic composites which have an important, and in many cases, a decisive influence on the integral mechanical properties of these materials is the interphase boundary. In this paper, based on numerical simulation we show the influence of morphology and strength properties of interfaces for integral mechanical properties of the dispersion-reinforced composite NiCr-TiC (50 : 50). Computer simulation results indicate that the phase boundary significantly contributes to the integral mechanical characteristics of a composite material and to the nature of the initiation and development of cracks.

INTRODUCTION

Sintered materials based on refractory and high hardness chemical compounds (carbides, nitrides, oxides) with metal binder are characterized by high values of mechanical and tribological characteristics such as strength, hardness, fracture toughness, wear resistance, and fracture energy. An effective way to increase the service life of metal-cutting tools includes modification of their surface layers up to 100 μm thick by pulsed high-energy electron beam irradiation in inert gas plasma [1]. This treatment is accompanied by partial dissolution and increase of the roundness of ceramic particles and formation of complex nanoscale structure of interphase boundaries. Thus, depending on the process parameters the mechanical properties of interfaces in the modified surface layers may vary widely. It is noteworthy that the interphase boundaries serve as a key element of the internal structure of composite materials, which has an important and, in many cases, a decisive influence on the integral mechanical properties of composites.

The nature of dependencies within mechanical properties of composites on the characteristics of the interphase boundaries, as a rule, is nonlinear and often non-monotonic. In this regard, to identify the type of dependencies and their generalizations for a wide range of dispersion-reinforced ceramic-metal materials computer simulation using multilevel models is widely used. A key structural level of such mesoscopic models is related to the scale of inclusions, in which the phase boundaries are treated as a separate structural element.

The aim of this paper is to develop a 3D numerical discrete model of mesoscopic metal-ceramic composite material, taking into account peculiarities of morphology and strength characteristics of interphase boundaries, and to study the laws of mechanical behavior of composites under uniaxial tension based on this model.

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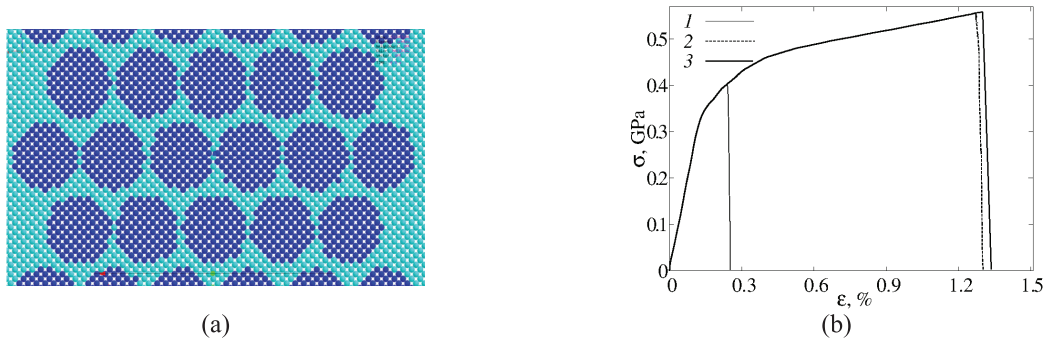

FIGURE 1. The structure of the modeled composite samples (a) and loading diagrams for the tension of composites with different strength of interphase boundaries (b). σ_B^{int}: *1*—$0.5\sigma_B^{NiCr}$, *2*—$1.0\sigma_B^{NiCr}$, *3*—$1.5\sigma_B^{NiCr}$

PROBLEM STATEMENT

For the construction of models of mesoscopic structural features of the interphase boundaries of composite we used two different approaches: 1) cohesive zone model (infinitely thin interphase boundary) [2]; 2) wide interface region surrounding ceramic particles. In the first case, we used a modification of non-potential model Zhubel–Baylor cohesive zone [3]. In this model, the resistance of the interface depends on a relative displacement of adjacent surfaces of two phases as a decreasing linear function. The second model is characterized by a finite width of interface region possessing their own mechanical properties (different from the matrix ones) such as yield strength and strain hardening parameter. It should be noted that traditional approaches to the definition of these parameters are based on the concept of geometrically necessary dislocations [4]. However, an additional change in the width and mechanical properties of the interface zones can be achieved by forming nanoscale internal structure, for example as a result of high-energy electron beam treatment.

As an object of the study, we considered cermet composite material based on NiCr matrix reinforced by dispersed TiC inclusions (50 vol %). It should be noted that in recent years the metal composite is the subject of a comprehensive study both experimentally [5, 6] and numerically [7–9].

The method of movable cellular automata [10] was used for numerical simulation herein. The advantage of this method for considered problem is the ability to investigate the mechanical response of the material, taking into account the processes of fracture (including multiple) and contact interactions formed surfaces.

Uniaxial tension experiments were conducted numerically on representative mesoscale volumes (samples) of the box shape (Fig. 1a). Disperse inclusions had a rounded shape and approximately the same dimensions of the order of 2.5 μm. In the description of interfaces using the cohesive zone model, interface strength (critical value of equivalent stress in the considered case) was considered as the model variable parameter. When using the model of hardened interface region, the model variable parameters were the yield strength and the strain hardening coefficient of interface zone.

Properties of the movable cellular automata modeling NiCr corresponded to experimental data for the alloy X20H80-H density ρ = 8400 kg/m^3, Young's modulus E = 217 GPa, Poisson's ratio ν = 0.300. As an input parameter for computing strength criterion based on the value of the equivalent stress, a table-valued uniaxial compressive strength of this material (σ_B = 834 MPa) was used. Properties of automata simulating TiC were set in accordance with the following experimental data: ρ = 4920 kg/m3, E = 439 GPa, ν = 0.188, σ_B = 1380 MPa.

SIMULATION RESULTS

Composite with Infinitely Thin Interfaces

As noted above, the main parameter of the mechanical interface described by the cohesive zone model is the value of strength. In this study, the value of interface strength σ_B^{int} varied in the range of $0.5\sigma_B^{NiCr}$ (low adhesion strength of NiCr matrix to TiC inclusions) to $1.5\sigma_B^{NiCr}$ (high adhesion strength due to, for example, the formation of nanostructured states on the border), where·σ_B^{NiCr} is the strength of NiCr matrix. Examples of loading curves for model sample uniaxial tension are shown in Fig. 1b for some values of σ_B^{int}. As seen from the figure, although the change in the interface strength has no effect on the magnitude of the effective elastic limit, however, provides a significant increase in the integral strength of the composite (up to 30%), as well as a multiple increase of its ultimate strain, and fracture energy (area under the loading curve). Note that when the value of the interface strength is equal to the strength of the matrix, the values of the integral strength and fracture energy of the composite tend to saturation and the further increase in strength of the interfacial boundaries practically produce no changes.

Analysis of the simulation results showed that when the interface strength is much less than the strength of the plastic matrix ($\sigma_B^{int} = 0.5\sigma_B^{NiCr}$), the destruction of the composite begins with the initiation of interface cracks in the area close to interfaces, the crack normal is coaxial with the loading direction. On further tension, the system of isolated interface microcracks is formed mainly in the center of the model sample, and gradually merges into a single main crack. Thus, in this case the failure occurs in the form of microcracks at the interfaces with the matrix and their subsequent incorporation by "links" passing through the plastic matrix.

When the strength of the interface exceeds the strength of the inclusion material $\sigma_B^{int} > \sigma_B^{NiCr}$), the failure pattern undergoes a qualitative change. In this case, the first microcracks isolated from each other are formed inside the inclusions. The preferred orientation of microcracks is perpendicular to the loading direction. On further tension, accompanied by the increase of internal stresses in the matrix, new microcracks are being generated which coalescence with the "primary" cracks in the volume of inclusions combines them into a single gap propagating across the sample mainly in the inclusions. Thus, in this case, failure also occurs in the direction perpendicular to the direction of loading, but the main crack passes predominantly through the inclusion and has an almost flat shape.

The revealed dependences of the composite failure pattern on the strength of interphase boundaries are consistent with the results of numerical simulation of various composite materials conducted by other authors [11, 12].

Composite with "Extended" Interphase Boundaries

Interface zone around the ceramic particle is formed during the production/processing of the composite due to formation of geometrically necessary dislocations and intensive processes of diffusion and/or mixing (in the case of the zone formation from the melt). Mechanical properties of the interphase transition zone (primarily, yield strength and strain hardening rate) may differ significantly from the properties of the metal matrix. The typical width of the interface zone is determined by the conditions of the composite production/processing, and varies from a few tens of nanometers to micrometers on. In this work, we carried out the analysis of the effect of mechanical properties of the interphase zone of submicron width (250 nm) in the mechanical response of model specimen of the metal-ceramic composite.

Figure 2a shows the response function of the movable cellular automata used for modeling interface zones with different values of the elastic limit σ_y^{int}. Note that the increase in the yield stress of interface material traditionally associated with the increase in the density of geometrically necessary dislocations due to mismatch of the coefficients of thermal expansion of the materials of matrix and inclusions. The degree of strain hardening of the interface material, in this case, is assumed to be equal to the same of the matrix.

Figure 3a shows the automaton response function for modeling interface zones with different values of both σ_y^{int} and K^{int}. Here is a special case of increasing the elastic limit and the strain hardening coefficient in the same proportion with respect to the relevant parameters of X20H80-H. Simulation shows that the change in rheological properties leads to an increase (a significant change in comparison with the elastic limit only, Fig. 2) of both strength and ultimate strain of the composite. Thus, by increasing the elastic limit strain hardening coefficient and a 20% strength alongside with the work of fracture of the composite is increased by 11 and 20%, respectively (Fig. 3b).

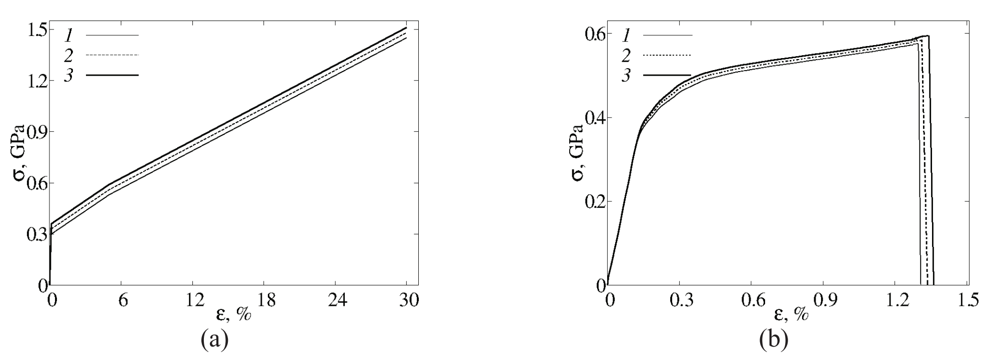

FIGURE 2. Response functions of the movable cellular automata used for modeling interface zone (a) and diagrams of uniaxial tension of the modeled samples of metal-ceramic composites (b) with interface zone characterized by different values of elastic limit σ_y^{int}: *1*— σ_y^{NiCr}; *2*—$1.1\sigma_y^{NiCr}$; *3*—$1.2\sigma_y^{NiCr}$

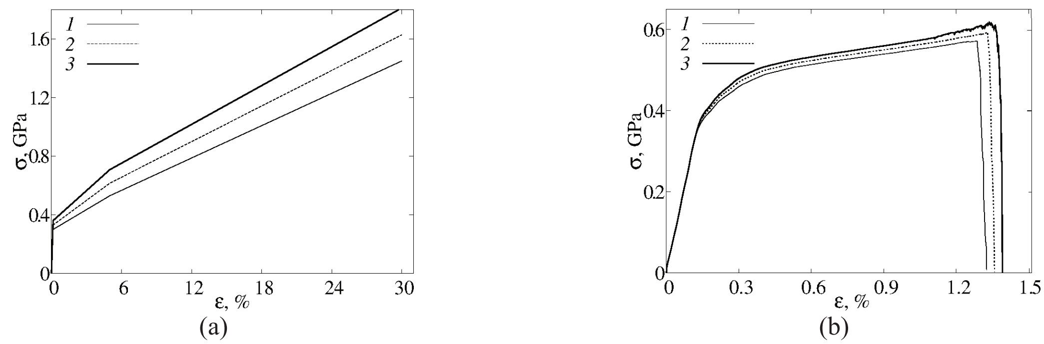

FIGURE 3. Response functions of the movable cellular automata used for modeling interface zone (a) and diagrams of uniaxial tension of the modeled samples of composites (b) with the interface zone characterized by different values of hardening coefficient K^{int}: *1*—$\sigma^{\mathrm{int}}{}_{y} = \sigma^{\mathrm{NiCr}}{}_{y}$, $K^{\mathrm{int}} = K^{\mathrm{NiCr}}$; *2*—$\sigma^{\mathrm{int}}{}_{y} = 1.1\sigma^{\mathrm{NiCr}}{}_{y}$, $K^{\mathrm{int}} = 1.1K^{\mathrm{NiCr}}$; *3*—$\sigma^{\mathrm{int}}{}_{y} = 1.2\sigma^{\mathrm{NiCr}}{}_{y}$, $K^{\mathrm{int}} = 1.2K^{\mathrm{NiCr}}$

CONCLUSIONS

Computer simulation results indicate that the phase boundary significantly contributes not only to the integral mechanical characteristics of the composite material but also to the nature of the initiation and development of cracks. The extent of this contribution is determined by the width of interfaces.

For cermet composite with "narrow" interphase boundaries, the increase in the interfaces strength determines the growth of the integral strength, ultimate strain, and fracture energy. It also causes the change in the failure pattern: for the composite with the interface strength below inclusions strength the failure occurs by partial inclusion delamination and integration of these cracks in a single gap. If the interface strength exceeds the strength of the inclusion material, the main crack is formed through the merger of damages formed in a number of inclusions. This main crack usually develops perpendicular to the direction of loading.

For composites with interphase boundaries of finite width, the increase in the mechanical properties of boundaries, including the elastic limit and strain hardening coefficient, causes an increase in the integral strength, ultimate strain, and fracture energy. At the same time the failure pattern does not undergo any significant changes, however, there is a tendency to increase the number of secondary cracks, feathering the main crack.

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