Simulation of Mechanical Loading by Cylindrical Indenter of "Ceramic Coating — Polycrystalline Metallic Substrate" Composition

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Abstract. In the present research a new hybrid multilevel approach was developed. It is shown that discrete-continual approach of excitable cellular automata can be successfully applied to simulation of deformation processes in systems with clearly pronounced interfaces. Explicit account of interfaces at various scales (interface between coating and substrate, grain boundaries etc.) allowed estimating power of stress concentrators to occur at these boundaries and also investigating specific features of stress field evolution in systems with coatings under dynamic compression by indenter.

Introduction

In spite of a lot of efforts to be undertaken for a long time in tribology, analysis of physical processes at contact interaction is still very actual and complex problem. At the same time it was discussed widely in literature [1-4]. Basic and very important features, which are characteristic for contact interaction of materials could be formulated in following way: a) simultaneous presence of several characteristic scales of deformation processes; interaction of processes at these scales determines a character of material response to this type of loading; b) specific role of interface, which takes a great part of loading being applied to a specimen; interface (like a filter) selectively transfers mechanical energy to deeper located layers.

It is necessary to note that, in spite of existance of a large number of models in mechanics of contact interaction, explicit account of evolution of internal structure of loaded specimen at various scale levels is still remained without proper consideration [5]. This problem is very actual because of development of new materials, where elements of internal structure play a determining role in evolution of plastic deformation and governs of pattern of fracture. In this case application of continuum mechanics is not always correct. Besides that, during friction and wear in a specimen under loading (especially in its surface layer), additionally to strain hardening, structure-phase transformations and recrystallization can occur; also nano- and micropores and cracks can be nucleated. These phenomena should be taken into account explicitly with the help of assignment of internal structure and its response onto external action. In that way, development of new approaches to simulation of processes of contact interaction and their following adaptation to investigation of processes of friction and wear of heterogeneous materials within the framework of multilevel approach is actual modern physical problem. For the solution of the latter it is necessary to work out new methods, which take into account in explicit form both structure of medium under simulation and specific features of interaction of structure elements. Such methods include discrete approaches. More developed discrete approaches are methods of molecular dynamics and cellular automata methods.

An approach to solution the problem is developed by the authors in present research in the form

of hybrid method of simulation. The proposed approach can be successfully applied to description of processes evolving under deformation and wear.
Methodological foundations of construction of multilevel model were developed in the framework of physical mesomechanics of materials [6]. In addition to that it was shown that account of thermodynamic stability of crystal lattice is of actuality. This stability is associated with the fact that a crystal tends to save its translation symmetry in fields of external actions. Detailed description of this approach is given in the work [7] based on consideration of the dependence of the thermodynamic Gibbs potential on the molar volume of a loaded material in a field of external forces.

Simulation of microindenter with the help of discrete-continual approach of excitable cellular automata

A solid as a multilevel hierarchical system under extreme external actions (mechanical, thermal, radiation etc.) experience structural-phase transformations at each scale. Evolution of these transformations can be represented in the form of flows of all kinds.
Continuum mechanics being a good tool for solution of applied tasks of elasticity theory at macroscale, did not initially aim at description of media with structure. Complexity of application of continuum mechanics methods to computer simulation of dynamics of internal material structure variation is associated with a lot of factors. One of the factors is the fact that in the framework of these tasks one should consider both presence of internal structure effecting on energy transfer and dynamic transformation of the structure and configuration of internal interfaces.
As a rule, existing approaches of continuum mechanics take into account presence of internal structure by means of assignment of so-called «nonlinearity of properties», i.e. spatial variation of parameters of medium simulated [8]. But during constructing of models in the framework of approaches of physical mesomechanics it is necessary to take into account both internal structure of material by means of assignment of different properties of separate elements (as in the framework of numerical methods of continuum mechanics) and hierarchical character of interaction of various structural elements.
In the present paper it is suggested to use discrete-continuous approach of excitable cellular automata (Stochastic Excitable Cellular Automata – SECA) for simulation of behaviour of multilayer structures under action of microindenter. In the framework of SECA method a specimen modelled is divided into elementary volumes, when each of them is simulated with the help of active element contained in cellular automaton. In doing so each element is characterized by certain set of neighbours at first coordination sphere and also by the numerical parameters corresponding to the material contained in simulated volume of space, such as the modulus of elasticity, the density, the shear modulus, the density of dislocations, the heat conductivity, the specific heat capacity, the coefficient of thermal extension etc. Under interaction with neighbour elements thermal and mechanical components of energy and corresponding physical parameters (the temperature, the entropy, the stress, the strain, the density and so on) can be changed.
Depending on the specific features of the process simulated the parameters of active element, whose change can lead to switching of element, are chosen. Under simulation of processes associated with flows and distribution of mechanical energy it is reasonable to establish correspondence between element states and stages of loading of a solid: elastic deformation, plastic deformation, prefracture, fracture. Switching of state can be realized both deterministically and stochastically. Depending on type of switching an automata can be deterministic and probabilistic. In the framework of the proposed SECA method cellular automaton is probabilistic, i.e. each value of investigated parameter is associated with certain set of values of probability of switch to a corresponding state.
Each element of excitable cellular automaton can come through a consecutive series of state switches under external impact. Under interaction of active element with neighbours thermal and mechanical components of energy can be changed that leads to change of corresponding physical parameters (the temperature, the entropy, the stress, the strain, the density etc.). Besides the

parameters to describe a material, the important characteristic of cellular automaton is the type of pattern of element packing, which determines the number of element neighbours at first coordination sphere and the topology of connections between them. The packing type determines a number of vectors of energy flows under interaction with neighbours.
Under deformation simulation it is supposed that some part of energy is spent for change of the density of each active element, and another component of energy – for increase of its entropy. According to the value of the total internal energy of each elementary volume one can obtain distribution of the normal components of the stress tensor in the whole specimen, including its surface, with the help of Murnaghan equations [9]. In details the fundamentals of SECA method are stated in [10-12].
It is necessary to note that in the framework of proposed approach boundary active elements are divided into three types: «hard», «soft» and «intermediate». «Hard» boundary elements do not change own energy under interaction with internal elements of specimen. Reciprocal action of such elements is not simulated. «Soft» boundary elements interact with all neighbours at first coordination sphere, both internal and boundary, and its energy varies according to the equations for energy flow. At last, «intermediate» boundary elements do not interact with neighbour boundary elements and change its energy as a result of effect of internal neighbour elements at first coordination sphere.
Together with the developed method of simulation of mechanical energy transfer possibilities of the model were extended by means of the algorithm of calculation of local couple forces appearing in complex loading schemes. The values of the principal stress of active element and the summary couple force applied to it are calculated according to the effective stress values of given element and its neighbours at first coordination sphere. The algorithms of calculation of the principal stress and the couple force are described in details in [13-14].
It is evident that design of modern structural materials is impossible without special technologies of modification their internal structure with the purpose of optimization of certain physical and mechanical characteristics necessary for achieving reliable and long-term service in conditions of extreme external actions. It is characteristic feature for materials with nanocluster structure especially. According to that, computer simulation of these materials without explicit account of internal interfaces as self-dependent subsystems does not correspond to modern level of requirements to models and methods for its realization.
Complex configuration of disordered atoms at intercluster boundaries effects essentially on character of transfer of mechanical and thermal energy parts. Properties of structural materials depend essentially on topology of intercluster boundaries, so models of structure design with possibility of explicit governing by the parameters of internal geometry of structure are necessary. Therefore in the purpose of explicit account of interfaces between structure elements the SECA method was developed for building three-dimensional model of grain structure generation by means of division of united cellular automaton into separate clusters. Each cluster is characterized by the set of Euler angles determining orientation of crystal lattice in the interior of the cluster.

Description of numerical experiments

It is known that forming of dispersed transition layer between coating and substrate (for example, by means of ultrasonic machining) can be very important factor for increase of wear resistance of such compositions [15]. For checking this suggestion two sets of numerical experiments were carried out. In the framework of these experiments an indenter loading of polycrystalline specimens with coatings were carried out. The first type of the coatings contained intermediate finely divided layer, the second type did not contain it.
SECA method used for calculations allows estimating the value of the uniform hydrostatic stress as the function of the elastic energy. The elastic energy is redistributed in a system of active elements of cellular automaton by means of transfer from «energy spot» imitating indenter at top facet of specimen. Each specimen was simulated by cellular automaton in the form of system of active

elements with the size 1 μm in face-centered packing. The sizes of the specimens were equal to 50 μm × 20 μm × 50 μm. In first set the specimens represented the composition «ceramic surface layer – coarse-grained aluminium alloy substrate». Second set of numerical experiments was purposed to simulate behaviour of the compositions «ceramic surface layer – fine-grained aluminium intermediate layer - coarse-grained aluminium alloy substrate». In first case the thicknesses of surface layer and substrate were equal to 10 and 30 μm respectively; in second case surface layer, intermediate layer and substrate had thicknesses equaling to 10, 10 and 30 μm respectively. The size of grain in fine-grained intermediate layer was equal to 3 μm, in coarse-grained substrate – 10 μm. The initial values of the stress and the strain were equal to zero for all cells. The time step was equal to 1 ns for all numerical experiments.
Boundary conditions to imitate indenter action were assigned for each specimen in the following way. In the centre of the top facet (on the coating surface) the area with the diameter 12 mcm was located. In this area the velocity of increase of the uniform hydrostatic stress to be equal to 380 GPa/s was assigned. At each time step distribution of the values of the stress, the strain and the local couple forces in the specimen was simulated. The total time period for each numerical experiment was equal to 1 ms. The specimen structures are represented at Fig. 1.

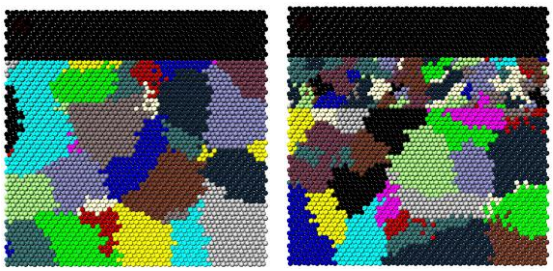


Fig. 1. Grain structures of the specimen without intermediate fine-grained layer (a) and the specimen with intermediate fine-grained layer (b): section by plane perpendicular to indenter.

At Fig. 2 evolution of fields of uniform stresses for two compositions «coating – coarse-grained substrate» and « coating – fine-grained intermediate layer - coarse-grained substrate» is represented. Due to discreteness of active elements of cellular automaton explicit account of grain boundaries in SECA method allows not only estimating a power of stress concentrators at the interfaces but calculating the value of the gradients of the stress and the strain along these boundaries.

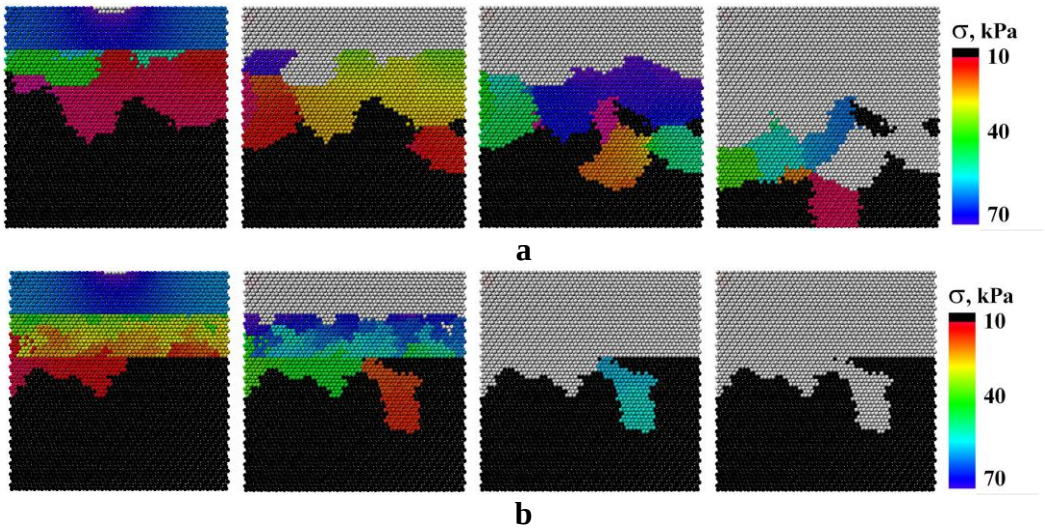
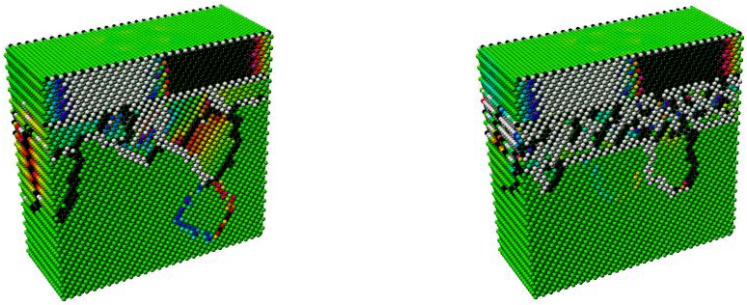


Fig. 2. Distribution of the stress values in plane of section at consecutive time moments at initial stage of the numerical experiment: a. the specimen without intermediate fine-grained layer; b. the specimen with intermediate fine-grained layer.

Comparison of the dynamics of changing the stress fields for these two structures gives a possibility to make a conclusion that the velocity of transfer of the elastic energy in the structure with the intermediate fine-grained layer (Fig. 2b) is essentially lower than that in the initial structure of the specimen with the coating (Fig. 2a). This fact indicates a damped role of the intermediate layer characterized by larger area of grain boundaries and smaller size of structure elements.

For investigation of mechanisms of elastic energy absorption under transfer of deformation front through fine-grained intermediate layer the analysis of the patterns of distribution of the local couple forces in each specimen (Fig. 3) was fulfilled. Firstly, comparison of the patterns of distribution of the local couple forces at Fig. 3 shows that the domain of extreme values of the couple forces propagates from up to the bottom facet of the specimen without the intermediate layer (see Fig. 3, left side), whereas in the specimen with the intermediate one extreme values of the couple forces are observed at upper and middle layers of the coarse-grained substrate (see Fig. 3, right side).



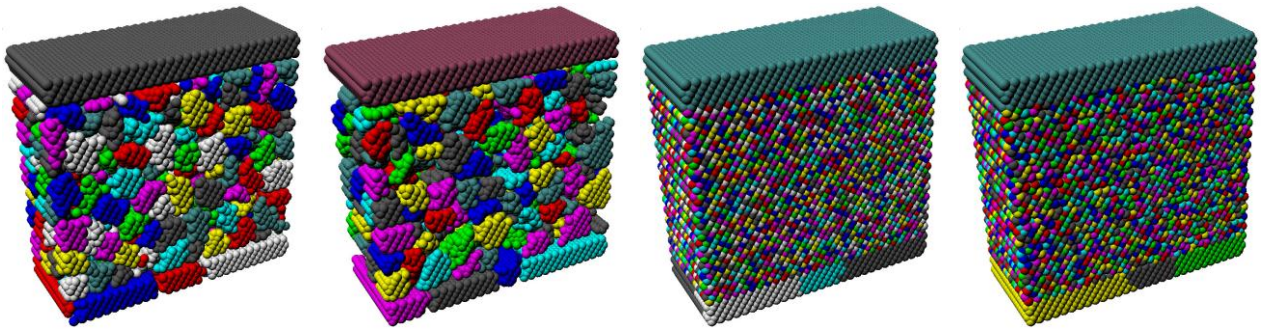
a **b**

Fig. 3. Distribution of the couple force values at lateral facets of the specimens without intermediate fine-grained layer (a) and with intermediate fine-grained layer (b).

Secondly, the distribution represented in Fig. 3b indicates a larger density of fluctuations of the couple force values with opposite signs in the intermediate layer. These fluctuations compensate each other by means of local shears and rotations of fine-grained structure that leads to absorption and dissipation of considerable part of the elastic energy. One can suppose that given process is one of the main reasons of damped character of the intermediate fine-grained layer.

Thus, presence of sharp interface between coating and coarse-grained substrate leads to larger depth of strain localization. Fine-grained structure of the intermediate layer allows redistributing the elastic energy of indenter by means of dispersing stress concentrators at larger area of internal interfaces and decomposition of the total strain on multiple shears and rotations of the structure elements.

For detailed investigation of processes of deformation front propagation and elastic energy transfer taking into account energy dissipation a series of numerical experiments on dynamic compression of specimens with coatings and various structure parameters was carried out. Each specimen represented a cellular automaton in the form of a system of active elements constituting face-centered close packing. The size of each active element was equal to 0,1 μm. In all series of the numerical experiments «aluminum oxide coating with internal structure elements of various sizes – hard aluminum alloy substrate» compositions were simulated. The specimens had size of $5 \times 2 \times 5$ μm. Upper layer of the specimen had the thickness 0,5 μm and imitated the indenter part effected by dynamic compression with the velocity 100 GPa/s. The coating thickness was equal to 4 μm, the thickness of the substrate layer equaled 0,5 μm. At each time step distribution of the values of the stress, the strain and the local couple force was simulated. The specimen structures are represented at Fig. 4.

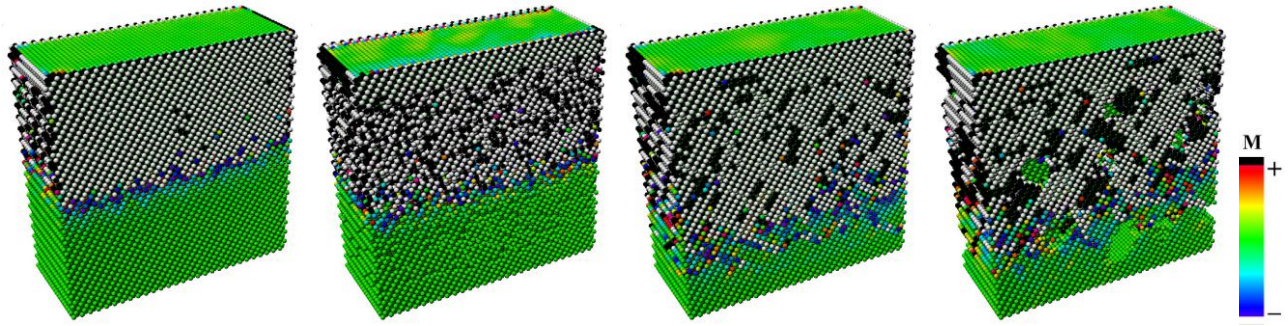


a **b** **c** **d**

Fig. 4. General view of the specimens simulated with the coatings of various structures: a. polycrystalline (d = 0.5 μm) oxide of aluminium; b. polycrystalline (d = 0.5 μm) porous oxide of aluminium; c. nanocrystalline (d = 100 nm) oxide of aluminium; d. nanocrystalline (d = 100 nm) porous oxide of aluminium.

In first series the composition «polycrystalline aluminium oxide coating – coarse-grained aluminium substrate» was simulated. Grain sizes in coating and substrate were equal to 0,5 μm (Fig. 4, a) and 1 μm (Fig. 4, c) correspondingly. In second series the specimens were the same as the initial composition but contained pores with the sizes 0.5 μm (Fig. 4, b) and 0.1 μm (Fig. 4, d) had the porosity equal to 10 % approximately.

In the present study authors fulfilled an analysis of distribution of the values of the local couple force formed in the coating as a result of inhomogeneous distribution of stresses among structure elements. Pictures 5, a, and 5, b, illustrate the patterns of distribution of the couple force values obtained in the numerical experiments for polycrystalline continuous and porous structures correspondingly.



a **b** **c** **d**

Fig. 5. Distribution of the couple force values (after 1 μs of the numerical experiment):a. in the specimen with polycrystalline coating (the grain size – 0.5 μm);
b. in the specimen with polycrystalline porous coating (the pore size – 0.5 μm);
c. in the specimen with nanocrystalline coating (the grain size – 0.1 μm);
d. in the specimen c nanoporous coating (the pore size – 0.1 μm).

One can see that regions of extreme values of couple forces of opposite signs in case of polycrystalline non-porous structure (Fig. 5, a) are distributed at grain boundaries. It indicates that in these regions powerful stress concentrators are formed and initiate defect flows along these boundaries. Later these flows can lead to generation of defects at higher scales to provide grain-boundary fracture pattern of the coating. At the same time, stress concentrators in porous structure (Fig. 5, b) are larger and can include the whole grain. It indicates that given structure can provide vortex character of deformation both along grain boundaries and in separate element of structure. Hence, one can make a conclusion that porous polycrystalline coating can be fractured both according to mechanism of grain-boundary sliding and by means of spalling of separate structure elements under rotations of grains because of their weak reciprocal connectivity. Investigation of

size effect of structure elements onto character of deformation front propagation and distribution of couple forces in coating was carried out. For this purpose compositions analogous to those used in the first two series of numerical experiments were simulated. In addition, the character sizes of structure elements and pores were five times less than initial ones (~100 nm). The composition structures are illustrated at Fig. 4, c, d.

Patterns of distribution of local couple forces in nanostructured coating show that front of inelastic deformation associated with irreversible character of action of shear stresses has propagated in the depth less than in case of coarse-grained structures (Fig. 5 c, d). It is necessary to pay attention to the following two facts. Firstly, in the framework of SECA method the local couple force includes both rotational and shear deformation modes. Secondly, modified Tornbull equation, which is initially responsible for mass transfer, is used for simulation of propagation of inelastic deformation front in SECA method. Thus, in the framework of the numerical experiments analyzed in this paper location of front of propagation of couple forces is the same that location of front of propagation of unconvertible shear strains.

Comparison of the patterns of distribution of couple forces for all these compositions allows making a conclusion that the velocity of inelastic shear deformation in the structure with nanoporous porous coating (Fig. 5, d) is less than in the specimen with coarse-grained coating (Fig. 5, a). This fact indicates damped role of porous nanostructure characterized by larger area of grain boundaries and smaller size of structure elements.

For investigation of mechanisms of absorption of elastic energy under deformation front propagation through coating analysis of dependences of the local couple force on the time was realized for each specimen (Fig. 6). Comparison of the graphs showed that in the specimen with nanostructured nanoporous coating of the sum of the absolute values of the couple force is higher than in another structures during the whole numerical experiment.

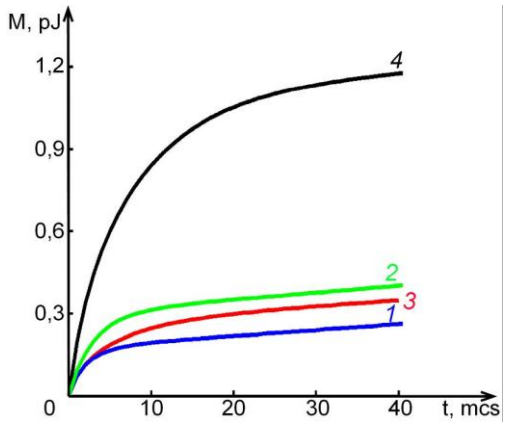


Fig. 6. Dependences of the sum of the absolute values of the local couple force for the compositions: 1 - in the specimen with polycrystalline coating; 2 - in the specimen with polycrystalline porous coating; 3 - in the specimen with nanocrystalline coating; 4 - in the specimen c nanoporous nanocrystalline coating.

On the other hand, couple force distribution for this composition (Fig. 5, d) indicates larger density of their value fluctuations of opposite sign in nanoporous nanocrystalline coating. Additional analysis of the values of the couple force sum taking into account its sign showed that these fluctuations compensate each other by means of local shears and rotations in polycrystalline structure, so that the vector sum of the couple forces is close to zero. It is evident that it leads to absorption and dissipation of considerable part of elastic energy.

Thus, process of permanent dividing of inelastic deformation front on set of vortices of smaller scale is one of the main causes of damped character of nanoporous structure of coating simulated in the last series of numerical experiments. Numerical experiments fulfilled on basis of SECA method

give a possibility to suppose that porous nanostructure allows absorbing a considerable part of elastic energy of external field of stresses generated by indenter. On the other hand, such structure promotes deceleration of growth of main crack that increases bearing capacity of the whole composite.

Summary

Investigation of dynamics of development of stress fields showed the possibility of damping of intermediate fine-grained layer between coating and substrate. The additional algorithm of calculation of the local couple force provided possibility of analysis of patterns of the couple force distribution in intermediate fine-grained layer and helped to explore the reason of decrease of velocity of elastic energy transfer through interlayer. It is shown that this decrease is associated with elastic energy dissipation during material shears along grain boundaries and rotations in fine-grained structure.

Thus, the simulation results showed that two factors play a governin role in elastic energy damping in fine-grained intermediate layer. The first factor is large area of grain boundaries; the second one is small grain size providing a possibility of realization of material rotations of structure elements. Numerical experiments based on SECA method allows supposing that, firstly, porous nanostructure of coating absorbs a considerable part of elastic energy of external stress field caused by indenter. Secondly, it is shown that such structure decelerates growth of main crack that leads to increase of bearing capacity of the whole composite.

In process of exploitation of compositions «coating - substrate» cracks can be generated. It is important to provide conditions when presence of these cracks does not lead to fast localization of deformation and transition of deformation at macroscale with following fracture. One of these conditions is relaxation of stored stresses. As it was clearly demonstrated by the numerical experiments, the effective relaxation of stresses can be provided by means of dissipation of elastic energy under compensating rotations in fine-grained structure.

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