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# ROLE OF VORTEX-LIKE MOTION IN CONTACT LOADING OF STRENGTHENING COATING. MOVABLE CELLULAR AUTOMATON MODELING

**ALEXEY YU. SMOLIN[1], GALINA M. EREMINA[2] AND SERGEY G. PSAKHIE[3]**

[1] Institute of Strength Physics and Materials Science
Siberian Branch of Russian Academy of Sciences
pr. Akademicheskiy 2/4, 634021, Tomsk, Russia
e-mail: asmolin@ispms.tsc.ru , web page: http://www.ispms.ru

[2] Tomsk State University
pr. Lenina 36, 634050, Tomsk, Russia
e-mail: rector@tsu.ru , web page: http://www.tsu.ru

[3] Tomsk Institute of High Technology Physics,
Tomsk Polytechnic University
pr. Lenina 30, 634050, Tomsk, Russia
e-mail: rector@tsu.ru , web page: http://www.tpu.ru

[4] Skolkovo Institute of Science and Technology (Skoltech)
Novaya St., 100, Karakorum Building, 4th floor, Skolkovo, 143025, Russia
e-mail: sp@ispms.tsc.ru , web page: http://www.skoltech.ru

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**Abstract.** Movable cellular automata (MCA) is an efficient numerical method in particle mechanics, which assumes that any material is composed of elementary objects interacting among each other according to many-particle forces. In this paper MCA method is applied to modeling deformation of 3D coating-substrate system under its contact loading by rigid indenter. Main attention of the research is focused on the role of vortex-like structures in the velocity fields in deformation of the strengthening coating and substrate. The mechanical properties of model coating correspond to multifunctional bioactive nanostructured film (TiCCaPON) and the properties of substrate, to nanostructured titanium. Loading is performed by hard conical indenter. The peculiarities of velocity vortex formation and propagation, as well as its interaction with structural elements are studied. One of possible application of the study is non-destructive technique for detecting nanoscale defects in surface layer of a material using frequency analysis of the force resisting to sliding of a small counter-body on the material surface, known as tribospectroscopy. Possibilities of this technique are studied based on 3D modeling by MCA method for the above mentioned coating with nano-pores. It is shown that specific peaks at the friction force spectrum correspond to different geometrical characteristics of the nano-pores.

## 1 INTRODUCTION

Dynamic loading of solids results in generation and propagation of surface elastic waves (Rayleigh and Love types) that have elliptical polarization and manifest themselves as vortex structures in the velocity field [1]. In thin plates such vortex structures are typical for Lamb waves [2]. It is known that during deformation of a heterogeneous material containing internal interfaces or/and free surfaces a collective vortex motion near these boundaries is formed [3]. For example, molecular dynamics simulations [4] show that vortex structures in the velocity field are formed at grain boundaries under shear loading of polycrystals [5]. Therefore, one should expect that rotational motion in nanomaterials takes place at different scales from the atomic scale to the macroscopic one. Results of theoretical studies and experimental evidence indicate that in nanomaterials the contribution of rotational mode of deformation can significantly increase under the condition of dynamic loading [6]. Nevertheless such a fundamental factor as elastic vortex motion in material formed during dynamic loading still remains out of discussion. A distinctive feature of the elastic vortex motion is its dynamic nature. It provides not only strain compatibility, but also serves as a mechanism of transfer and redistribution of elastic energy in the bulk of material and determines many features of the deformation process.

The above mentioned confirms that revealing the role of vortex displacement in redistribution of elastic energy and, as a result, in the process of deformation and fracture of nanomaterials is a topical fundamental problem in mechanics of nanostructured materials and materials science.

Due to principal significance of free surface, internal interfaces and dynamic nature of the considered vortex phenomena the main method of studying them seems to be computer modelling based on particle methods [7]. Therefore, the aim of this paper is revealing the role of vortex displacements in the contact interaction of strengthening coating with hard counter-body by means of 3D modelling using movable cellular automata.

We modelled brick samples of a coating under contact loading by a conical counter-body which moved along the upper surface of the coating. The bottom surface of the coating was fixed. The vector field of particle velocities as well as force of interaction between the counter-body and the coating were analysed. To detect vortices in the vector field we plot streamlines of the velocities vectors at different times. Note, that these streamlines show just a tendency of the particle motion not their real trajectories. Nevertheless, such an approach allows detecting position and measuring “power” of the vortex structures in 3D vector field of velocities.

A practical application of this study might be identification of defects in surface layers of materials based on measuring and analysing friction force (so called tribospectroscopy method [8]). That is why we also considered the peculiarities of vortices generation and propagation in case of presence of nanoscale pores and inclusions in the coating.

## 2 DESCRIPTION OF THE MODEL

For modelling interaction of a small counter-body moving over the coating surface we used movable cellular automaton (MCA) method, which is a new efficient numerical method in particle mechanics. Within the frame of MCA, it is assumed that any material is composed of a certain amount of elementary objects (automata) which interact among each other and can rotate and move from one place to another, thereby simulating a real deformation process [9]. The automaton motion is governed by the Newton-Euler equations. The forces acting on automata are calculated using deformation parameters, i.e. relative overlap, tangential displacement and rotation, and conventional elastic constants, i.e. shear and bulk moduli. A distinguishing feature of the method is calculating of forces acting on the automata within the framework of multi-particle interaction [10], which among other advantages provides for an isotropic behaviour of the simulated medium. Moreover, stress tensor components can be calculated for the automaton taking into account all the forces acting on it, which enables realization of various models of elastic and plastic behaviour developed in the frame of continuum mechanics.

A pair of elements might be considered as a virtual bistable cellular automaton (bonded and unbonded states), which permits simulation of fracture by the MCA. Switching-over of a pair of automata to an unbonded state would result in a changeover in the forces acting on the automata; in particular, they would not resist moving away from one another. Removing of automata from initial dense packing allows explicitly account of voids or pores in material. Changing sort (i.e. mechanical properties) of automata in initial packing allows account of various kind of inhomogeneity in the material.

In this paper the coating of multifunctional bioactive nanostructured film (TiCCaPON) on nanostructured titanium substrate [11] has been modelled (Figure 1,a). These materials are used in medicine for producing various kinds of implants. The thickness of the model coating is $H = 60$ nm. The model sample length $L = 350$ nm, width $M = 250$ nm, the size of the automata $d = 3$ nm. Diamond counter-body has a conical shape with a base diameter of 60 nm. We use cubic packing of automata, which is much more suitable for studying elastic deformation of the material due to less number of automata in the model and more uniform shape of the crack-like defects.

Motion of the counter-body is simulated by setting the constant velocity $V = 5$ m/s in the direction of axis $Y$ for automata of the upper layer of the counter-body (Figure 1,a). The lower surface of the sample is fixed and its lateral surfaces are free. When the counter-body is moving the resistance force of its movement on the surface is registered and associated with the friction force $F$ varying in time $t$. The Fourier transform is made for the registered friction force $F(t)$ and the corresponding spectra are analysed in order to study the influence of internal structure of the material and velocity field on the dynamics of friction force [12].

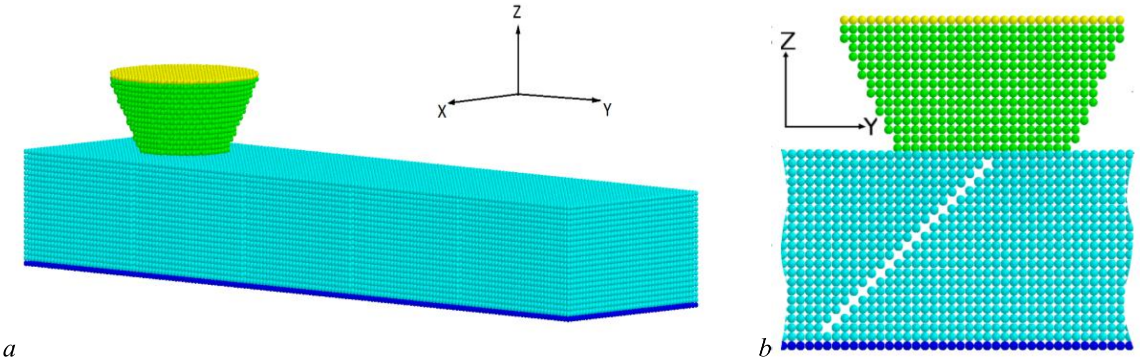


**Figure 1**: General view of the modelled system (a) and cross-section of the coating with a pore (b)

## 3 MODELLING RESULTS

Main attention of this research is focused on the role of vortex-like structures in the velocity fields in deformation of the strengthening coating and substrate. That is why first we studied the peculiarities of the velocity field in homogeneous coating under contact loading with hard conical counter-body moving along the free upper surface. Due to artificial roughness caused by discrete representation of the material and its surface, the movement of the counter-body along the surface with constant velocity results in periodic loading of the coating surface right in the contact patch. This cause generation of elastic waves in the coating, which propagate in the bulk and along the surface, and interact with another waves and structure elements of the material. As a result, the velocity field in the coating is drastically non-uniform and time dependent.

Analysis of numerical 2D vector field is very easy, one can see vortices in this case right from the picture of vectors shown as arrows or lines. Analysis of 3D fields is much more complicated problem. Evidently, one can try to look at 2D vector fields in a series of parallel sections of the 3D body. But, to see a vortex in this case you need to make sections by planes perpendicular to the direction of vorticity vector of the field (Figure 2,a). This means that first you need to compute the vorticity. But, the vorticity may have different orientations in different points; that is why this is not a right way. From the other hand, vorticity analysis is a typical task in hydrodynamics, and there are special tools in the computational fluid dynamics software for visualizing vortices. To analyse vorticity of the 3D vector field we used post-processor software VisIt [13]. To find vortices we plot streamlines of the velocity field at characteristic time steps (Figure 2,b). To make picture clearer we try different options and select the optimal ones. Of course, the resulting streamlines show just a tendency of the particle motion at the current time step, not real trajectories like in fluid dynamics. Nevertheless, this approach allows detecting position and "power" of vortex structures in 3D vector field of velocities and therefore is quite applicable for our task.

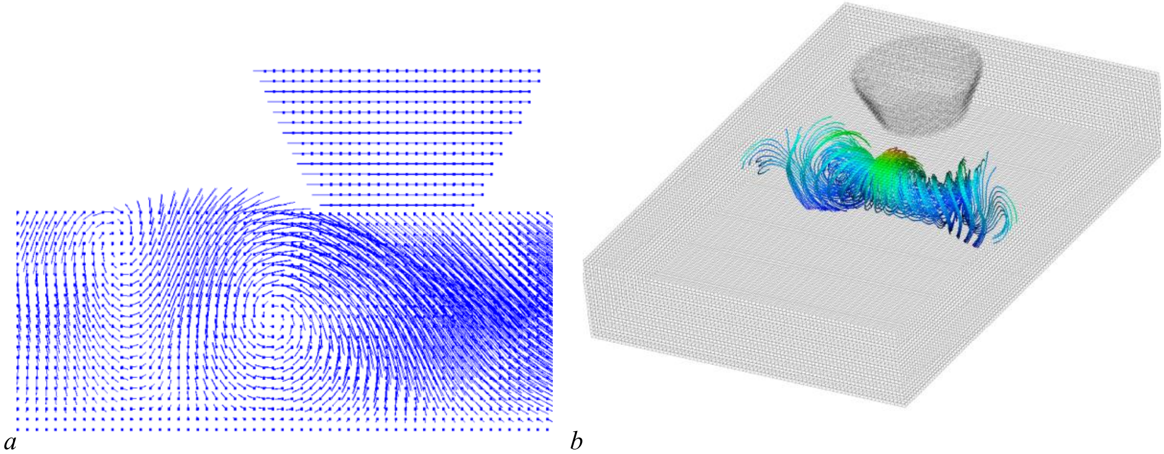


**Figure 2**: Vortex in the velocities of coating particles in front of the moving counter-body shown in cross-section of the sample (*a*, 2D picture) and in streamlines of the velocity field in 3D (*b*)

The peculiarities of velocity vortex formation in intact coating are as follows. Mainly, vortices occur in the corners of the coating, and are results of relaxation of elastic energy near free surface where it is allowed to move in several directions. But we tried to pay our attention to the vortices in the vicinity of counter-body. This vortex is formed periodically in time in front of the counter-body, and then it becomes wider, propagates ahead and rounds the counter-body. Lifetime of such vortex structure is about 0.015 ns, which corresponds to the time of sound propagation through the coating height. The vortex size is commensurable with half of the coating height.

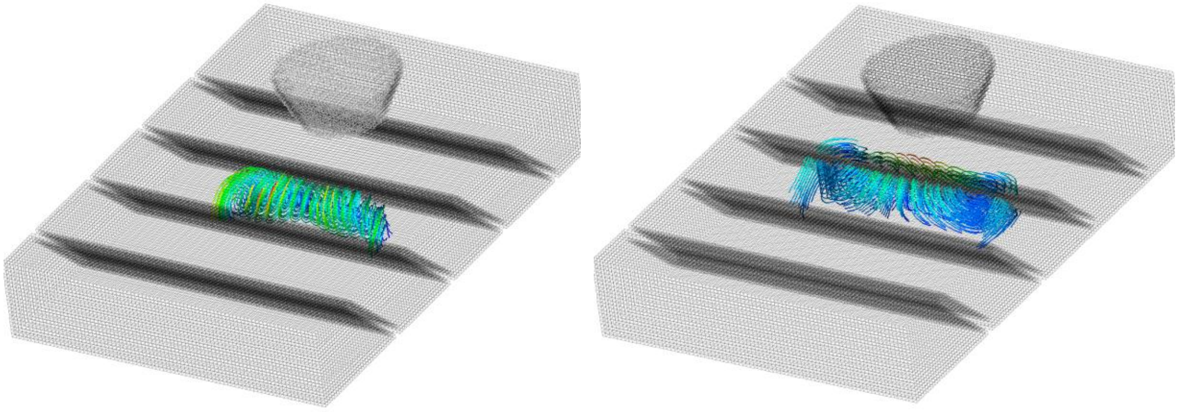

*a* *b*

**Figure 3**: Streamlines showing the vortices in the particles velocities of coating with pores (*a*) and hard inclusions (*b*)

Then we considered coating containing damages. The damage of the coating was simulated by specifying the extended discontinuities, nano-pores. These nano-pores were located periodically at the predetermined distance from one another and inclined to the upper surface by 45° (Figure 1,b). In this case vortex-like motion takes place only in the material between the pores and due to their specific geometry the vortex axis cannot round about the counter-body (Figure 3,a). The size of the vortex is less than one in case of intact material. The vertex is generated approximately in the middle of height of the coating. Then it becomes larger, propagates towards the lower surface along the orientation of the pores, and finally is divided into two parts which start to propagate to the right and left lateral surfaces of the coating correspondingly and vanishes. Lifetime of the vortex is the same as for the case of intact material.

The third coating sample modelled in this study contained hard inclusions of the same geometry as the pores in the sample of second type. Elastic properties of the inclusions are two times greater than elastic properties of the coating. That means that sound velocity in the material of inclusions is approximately 1.4 times greater than that of the coating. Typical vortex in the sample with hard inclusions is shown in Figure 3,b. One can see that it is similar to the case of intact material, but a little bit smaller.

One possible application of the study is non-destructive technique for detecting nanoscale defects in surface layer of a material using frequency analysis of the force resisting to sliding of a small counter-body on the material surface, known as tribospectroscopy [12]. When the counter-body is moving the resistance force of its movement on the surface is being recorded and correlated with the friction force $F$ varying in time $t$. The Fourier transform is made for the registered friction force $F(t)$ and the corresponding spectra are analysed. Here, the possibilities of this technique are studied based on 3D modelling by MCA method for the above mentioned coating with nano-pores and inclusions.

The Fourier spectrum for the inclined nano-pores (Figure 1,b) are shown in Figure 4,a. They have peaks characterizing the distance between the damages calculated by the formula proposed in [14]:

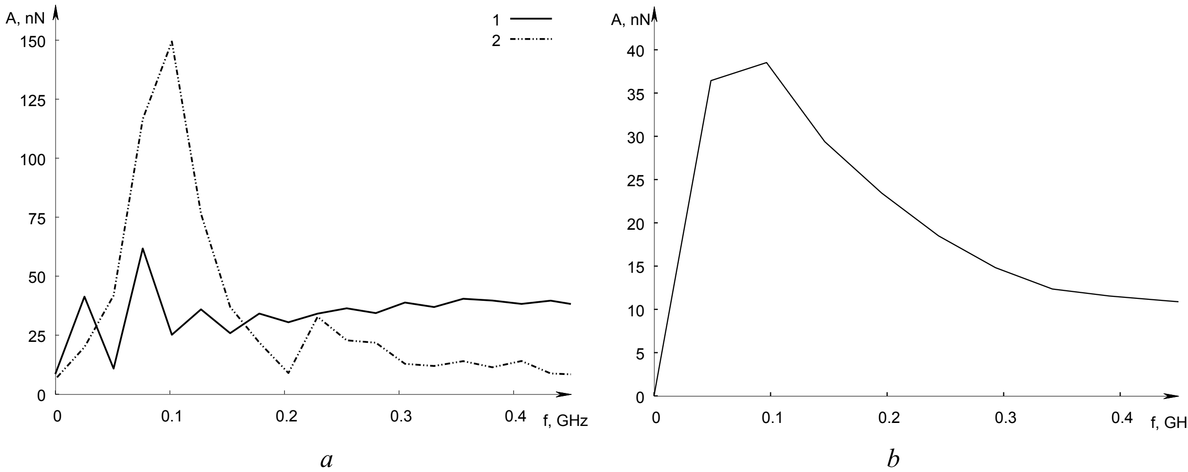
$$f = V/(P - D) \tag{1}$$

where $V$ is the velocity of the counter-body, $P$ is the distance between pores, $D$ is the diameter of contact area of conical counter-body with coating. For the specimen with the distance between the nano-pores equal to 96 nm this frequency is 0.128 GHz, and for the specimen with distance between pores 78 nm it is 0.277 GHz.

On the spectrum, one more peak at the frequency of 0.089 GHz occurs that is characterized by the following relation:

$$f = V/a \tag{2}$$

where $a$ is the projection of the nano-pore to the testing surface.



*a* *b*

**Figure 4**: Fourier spectra of the force $F(t)$ acting on the counter-body moving along coating with inclined nano-pores (*a*) spaced at 1) 96 nm and 2) 78 nm from each other; and with hard inclusions spaced at 96 nm (*b*)

The spectrum for the coating with hard inclusions is shown in Figure 4,b. One can see that it has a peak corresponding to the size of inhomogeneity and the distance between them. But in general the curve is smoother and has no peak, corresponding to the projection of the inclusion to the testing surface defined by Equation 2. It may be explained by the specific features of the vortex behaviour in case of presence of the pores. Namely that in this case the vortex propagates between the pores.

## 4 CONCLUSIONS

- A numerical model for studying peculiarities of vortex-like motion in contact loading of strengthening coating by hard counter-body has been developed based on movable cellular automaton method.
- To study vortex structures in 3D numerical velocity field a series of streamline pictures of the vector field at different time steps is analysed as well as vectors in plane slices of different orientation.
- Modelling results show that a counter-body sliding on the coating surface generate periodically vortex structures in velocity field of the coating. Each of these vortices is located in front of the counter-body at distance of the radius of contact area. Lifetime of the vortex is about the time of sound propagation through the height of the coating. After this time the vortex vanishes, and then after certain time appears again.
- Presence of pores and hard inclusions can change the shape and size of the vortex.
- We assume that such vortices play significant role in friction force dynamics that may be very important for tribospectroscopy method of detecting damages in surface layers of material.

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