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Modeling fracture of nanostructured bioactive coatings on Ti-based materials under contact loading

Alexey Smolin[a,b,*], Galina Eremina[b], Sergey Psakhie[a,b]

[a] *Institute of Strength Physics and Materials Science SB RAS, pr. Akademicheskii 2/4, Tomsk 634021, Russia*
[b] *Tomsk State University, pr. Lenina 36, Tomsk 634050, Russia*

Abstract

Modeling deformation and fracture of bioactive coating on Ti-based material is performed using movable cellular automaton (MCA) method. MCA is a new efficient numerical method in particle mechanics, which assumes that any material is composed of a certain amount of elementary objects interacting among each other according to many-particle forces. The mechanical properties of the model coating correspond to multifunctional bioactive nanostructured film (TiCCaPON) and the properties of the substrate correspond to nanostructured titanium. First, MCA method is applied to modeling nanoindentation of the coating. Indentations of diamond Berkovich tip for different depth of penetration are studied. The second testing technique which is considered for simulation using MCA method is a scratch test, in which an indenter moves across the surface after penetration. The third technique is an impact loading test. This test assumes periodic penetration of spherical counter-body into a coating with velocity about 10 m/s which leads to fracture of the coating. The calculation results are compared with available experimental data.

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1. Introduction

An effective method for enhancing the functional properties of materials is the application of special coatings to their surface. Thus due to the multicomponent nanostructured coatings based on refractory TiC and (Ti,Ta)(C,N) compounds, which contain special additions, i.e. Ca, Zr, Si, O and P, the quality of implants is upgraded and the tribological and bioactive properties of the implant surface are enhanced significantly Shtansky et al. (2004); Levashov et al. (2011). It should be noted that such coatings are in a nanosructured state; besides, they have small thickness. To date the investigations of mechanical properties of such coatings and films is generally performed by the nanoindentation method and scratch test Oliver and Pharr (1992); Shugurov et al. (2008). Nanoindentation is a process of controlled penetration of the superstrong instrument tip into the flat sample surface under increasing loading to a depth of 100 nm, with the force P acting on the indenter and the depth of penetration of the indenter tip into the

* Corresponding author. Tel.: +7-382-228-6975 ; fax: +7-382-249-2576.
E-mail address: asmolin@ispms.tsc.ru

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material, h, being measured continuously Levashov et al. (2011); Oliver and Pharr (1992). Using $P-h$ curve, the elasticity modulus, nanohardness and elastic recovery are determined for the material by the conventionally employed method of Oliver and Pharr (1992). However, it is shown by Shugurov et al. (2008) that a correct definition of the characteristics by the latter method is only feasible provided for the coating and the substrate having similar characteristics. Evidently, in the most important practical implementations this condition is not fulfilled. One of the methods of attack to address this problem is computer simulation which enables one to get sufficiently correct solutions regarding indentation of coatings on substrates of different kinds.

Scratch test technique involves generating a controlled scratch with a sharp superstrong tip on a selected area Flores et al. (2008). The tip is drawn across the coated surface under constant or progressive load. This allows quantifying friction and adhesive strength of the coating.

At present a lot of numerical studies of nanoindentation and scratching have been published. Depending on the method used for simulation they can be divided into two groups. The papers of the first group use the finite element method and consider behavior of the material at macroscale Dao et al. (2001); Bucaille et al. (2001); Makarov et al. (1998). The second group of the papers uses molecular dynamics (particle method) to study micromechanisms of plastic deformation nucleation in the vicinity of the indenter tip at microscale Zimmerman et al. (2001); Saraev and Miller (2006).

A numerical model based on particle method is proposed herein for description of the TiCCaPON coating on Ti substrate at meso- and macroscale. To make it possible we need a method that allows simulation of elastoplastic deformation and fracture of a solid at different scales. The best capabilities for modeling fracture, including crack growth and material fragmentation, belong to particle methods originated from molecular dynamics. Among the particle methods only the movable cellular automaton (MCA) method can describe plastic deformation correctly Psakhie et al. (2011, 2013). That is why it is chosen for this study.

2. Method of Movable Cellular Automata

MCA is a new efficient numerical method in particle mechanics that is different from methods in the traditional continuum mechanics. Within the frame of MCA, it is assumed that any material is composed by a certain amount of elementary objects (automata) which interact among each other and can move from one place to another, thereby simulating a real deformation process. The automaton motion is governed by the Newton-Euler equations:

$$\begin{cases} m_i \dfrac{d^2\vec{R}_i}{dt^2} = \displaystyle\sum_{j=1}^{N_i} \vec{F}_{ij}^{pair} + \vec{F}_i^{\Omega} \\ \hat{J}_i \dfrac{d^2\vec{\theta}_i}{dt^2} = \displaystyle\sum_{j=1}^{N_i} \vec{M}_{ij} \end{cases}, \tag{1}$$

where $\vec{R}_i$, $\vec{\theta}_i$, m_i and $\hat{J}_i$ are the location vector, rotation vector, mass and moment of inertia of ith automaton respectively, $\vec{F}_{ij}^{pair}$ is the interaction force of the pair of ith and jth automata, $\vec{F}_i^{\Omega}$ is the volume-dependent force acting on ith automaton and depending on the interaction of its neighbors with the remaining automata. In the latter equation, $\vec{M}_{ij} = q_{ij}(\vec{n}_{ij}\times\vec{F}_{ij}^{pair}) + \vec{K}_{ij}^{rot}$, here q_{ij} is the distance from the center of ith automaton to the point of its interaction ("contact") with jth automaton, $\vec{n}_{ij} = (\vec{R}_j - \vec{R}_i)/r_{ij}$ is the unit vector directed from the center of ith automaton to the jth one and r_{ij} is the distance between automata centers, $\vec{K}_{ij}^{rot}$ is the torque caused by relative rotation of automata in the pair.

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 MCA method is calculating of forces acting on the automata within the framework of multi-particle interaction Psakhie et al. (2011), which provides for an isotropic behavior of the simulated medium regarded as a consolidated body rather than a granular medium. Moreover, stress tensor components can be calculated for the automaton taking into account all the forces acting on the automaton Psakhie et al. (2011), which enables realization of various models of plasticity behavior developed in the frame of continuum mechanics.

A pair of elements might be considered as a virtual bistable cellular automaton, which permits simulation of fracture by the MCA. In this work a fracture criterion based on critical value of strain intensity was used. Switching of a pair