Three-Dimensional Movable Cellular Automata Simulation of Elastoplastic Deformation and Fracture of Coatings in Contact Interaction with a Rigid Indenter

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Abstract—The paper considers 3D movable cellular automata (MCA) models of contact interactions involved in nanoindentation, sclerometry, and tribospectroscopy. The system under study is a titanium substrate with a hardening coating. The substrate and coating materials are both described in the elastoplastic approximation. It is shown that the MCA method of numerical simulation provides correct description of the contact interaction of elastoplastic materials under different types of loads with explicit account for fracture. The possibility to detect damages in material surface layers from friction force estimates is assessed.

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1. INTRODUCTION

The contact problem of two elastic solids was solved for the first time by H. Hertz in 1882 [1]. Later, the theory of functions of complex variable allowed solving more complex contact problems taking into account the presence of discontinuities and voids in a material, viscoelastic and plastic properties, surface roughness (multiple contact), adhesion, etc. [2–4]. The present paper reports on computer simulation of contact interaction involved in nanoindentation, sclerometry, and tribospectroscopy as modern methods of measuring the hardness, strength, and other mechanical characteristics of material surface layers. The computer simulation is performed for materials with hardening coatings.

Coating deposition on materials is an efficient way of enhancing their functional properties. For example, implants are deposited with multicomponent bioactive nanostructured coatings based on TiC, (Ti,Ta)(C,N) refractory compounds added with special elements (Ca, Zr, Si, O, P) to improve their tribological and bioactive surface properties [5–8]. These coatings feature a nanostructural state and small thickness.

The mechanical properties of coatings and films are studied for the most by nanoindentation [9–12] and sclerometry [13–15]. Nanoindentation represents controlled penetration of a superhard tip (indenter) into the surface of material. Sclerometry (scratch testing) is a measuring process in which an indenter, when penetrated into the surface of material, moves along the coating resulting in its fracture. Among the nondestructive methods of coating quality control is tribospectroscopy [16]; this method allows detection of defects in coatings through measuring and analyzing the friction force induced by a small counterbody moving along the surface of material.

The foregoing processes are of both fundamental and practical interest. In theoretical terms, this is because their correct studies require development and improvement of computation techniques, thus generating a need for new numerical (computer) simulation methods. In terms of practical applications, interest in the processes owes to the advent of new materials specific in their composition, mechanical properties, and structure.

By now, numerical simulation of nanoindentation and scratching has been addressed in many papers. These pa-
pers, as regards the methods used, can be divided into two
groups. Works of the first group use the finite element
method and consider the behavior of materials on the
macroscale. In these works, the peculiarities of stress dis-
tributions in a material are studied depending on the in-
denter shape, mechanical properties of the material, etc.
[17–20]. The other group of works uses the molecular dy-
namics method (particle method) and studies the micro-
scale mechanisms of plastic strain nucleation in the im-
mediate vicinity of the indenter tip [21–24].

The objective of our work is to develop a particle mo-
del for describing the macroscale mechanical behavior of
a hardening coating on a metal substrate in contact inter-
action with a rigid indenter. Realizing this model requires
a method that would allow simulation of both elastopla-
tic deformation and fracture at different scales. The best
capabilities for simulation of fracture, including crack
nucleation and growth, fragmentation and mixing of mat-
ters, are offered by particle methods originating from mo-
lecular dynamics. It should be noted that of all such meth-
ods only the movable cellular automaton (MCA) method
provides correct description of plastic deformation of con-
solidated solids [25]. It is for this reason that the
MCA method is used to develop the desired model.

2. MODEL DESCRIPTION

The MCA method [25–29] is an efficient numerical
technique based on the concept of discrete elements (par-
ticles) which differs greatly from the concept used in nu-
merical methods of classical continuum mechanics. Dis-
crete methods have their origin in molecular dynamics
which allows atomic studies of materials. However, ato-
mic description is substantially limited in its possibilities
to cover spatial and temporal scales that are of interest for
engineering applications. This has led to the develop-
ment of methods similar to molecular dynamics but oper-
ating with meso- and macroscales—particle methods in
which structural elements have finite sizes (unlike atoms
being point masses) and interact only with the nearest
neighbors. The most well-known representative of this
method is the discrete element method [30–34], which is now widely used for studying the mechani-
cal behavior of granular (loose) and weakly bound me-
dia, in particular, rheological peculiarities of these sys-
tems, their fracture and mixing [32, 34]. At the same
time, until recently the discrete element method has been
applied mainly to study brittle porous materials [30–32,
34] due to insufficiently developed mathematical models
for calculating the interaction forces of discrete elements.
In particular, most of discrete element models use pair
(two-body) potentials or forces. This simplification pro-
duces a series of artificial effects, such as anisotropy, pack-
ing-imposed shear modulus and Poisson’s ratio, etc., in
the behavior of a particle ensemble [30, 34]. Among the
problems arising from these artificial effects is inadequa-
ty simulation of irreversible strain accumulation (plastic-
ity) in materials.

Recent studies show that many problems of the dis-
crete particle method, including those involved in de-
scription of consolidated solids, can be solved by using
many-body forces. According to the generalized ap-
proach [25], many-body forces for discrete elements can
be expressed on the same idea as interatomic potentials
are expressed in the embedded atom method. So, the for-
ce acting on a discrete element \( i \) with \( N_i \) neighbors can be
written as

\[
F_i = \sum_{j=1}^{N_i} F^\text{pair}_{ij} + F^\Omega_{i}.
\]

This force represents a superposition of the pair com-
ponents \( F^\text{pair}_{ij} \) dependent on the spatial position of the
automaton \( i \) relative to its neighbor \( j \) and the volume-depen-
dent component \( F^\Omega_{i} \) due to collective effects of the sur-
rounding.

The MCA method assumes that any material consists
of a certain number of finite-size elementary objects (au-
tomata) which interact with each other and can move in
space, thereby modeling real deformation processes. The
motion of automata is described by the Newton–Euler
equations:

\[
\begin{align*}
\frac{d^2 \mathbf{R}_i}{dt^2} &= \sum_{j=1}^{N_i} F^\text{pair}_{ij} + F^\Omega_i, \\
\frac{d^2 \mathbf{\theta}_i}{dt^2} &= \sum_{j=1}^{N_i} M_{ij},
\end{align*}
\]

where \( \mathbf{R}_i, \mathbf{\theta}_i, m_i, \) and \( \dot{\mathbf{J}}_i \) are respectively the radius-
vector, rotation vector, mass, and inertia moment of the
automaton \( i \); \( F^\text{pair}_{ij} \) is the pair interaction force of the
automata \( i \) and \( j \); \( F^\Omega_{i} \) is the volume-dependent force acting
on the automaton \( i \) due to interaction of its neighbors with
other automata. In the latter equation, we have \( M_{ij} =
q_{ij} (\mathbf{n}_{ij} \times F^\text{pair}_{ij}) + \mathbf{K}_{ij}, \) where \( q_{ij} \) is the distance from
the centre of the automaton \( i \) to the point of its interaction
(contact) with the automaton \( j, \) \( \mathbf{n}_{ij} = (\mathbf{R}_j - \mathbf{R}_i)/r_{ij} \) is the
unit orientation vector of the pair and \( r_{ij} \) is the center
distance of the automata (Fig. 1), \( \mathbf{K}_{ij} \) is the torque due to
relative rotation of the pair automata (see below).

Note that pair automata can represent parts of differ-
ent solids or one consolidated solid. Therefore, their in-
teraction is not always contact in the sense of the well-