Simulation of surface topography with the method of movable cellular automata

A.I. Dmitriev, V.L. Popov, S.G. Psakhie

Abstract

Development of surface topography of two solids in a frictional contact is studied with the method of movable cellular automata. After the running-in process, the bodies are separated and the surface power spectra of both bodies are determined. The power spectra show a dependence on the wave vector, which is typical for fractal surfaces. It is shown, that roughness parameters of friction surface depend on relative velocity of sliding and external pressure.

Keywords: Friction; Wear; Quasi-fluid layer; Surface topography; Fractal surfaces

1. Introduction

The microscopic processes at the interface between two solids in friction involve very different processes both in the surface layers of solids (plastic deformation, storage of damages, detaching of wear particles and their repeated welding into the surfaces) and in the intermediate medium (lubrication fluids, wear particles, products of chemical reactions of the bulk material with atmosphere and lubricants). The intermediate medium has neither the properties of solids nor of the fluid and is usually referred to as a ‘third body’ [1,2]. The third body develops often in such a way that the minimum energy dissipation in friction is provided [3,4].

In the present paper, we numerically investigate the formation of an intermediate layer between two solids in friction due to processes of plastic deformation, fracture and micro welding. For this purpose we use the method of Movable Cellular Automata—MCA. The MCA method allows to simulate such processes as plastic deformation, storage of micro damages and fracture, friction and wear, diffusion, adhesion, phase transformations and chemical reactions [5–8].

The modeled system is represented in the MCA method as an assembly of discrete elements—‘movable cellular automata’. The interactions of elements are defined in such a way that the isotropy of elastic properties is provided. Automata are characterized by the tensor of plastic deformation and the coupling state with their immediate neighbors. The parameter of the system are density, elastic constants, yield stress, fracture stress, fracture strain and viscosity.

The spatial evolution of movable automata is governed by the Newton–Euler equations of motion. This system contains both equations for translations and rotations:

\[
\begin{align*}
    m \frac{d^2 \vec{R}^i}{dt^2} &= \sum_j \left( \vec{F}^{ij}_n + \vec{F}^{ij}_r \right) \\
    \vec{J}^i \frac{d^2 \vec{\theta}^i}{dt^2} &= \sum_j \vec{K}^{ij}_r
\end{align*}
\]

where \( \vec{R}^i \) is radius vector; \( \vec{\theta}^i \), rotation angle; \( m^i \), mass and \( \vec{J}^i \), moment of inertia of an automaton \( i \), \( \vec{F}^{ij}_n \) and \( \vec{F}^{ij}_r \), normal and tangential force correspondingly. \( \vec{K}^{ij}_r \), moment of tangential force.

Each movable automaton is further characterized by a set of mechanical parameters corresponding to mechanical properties of the simulated material. The formalism of the movable cellular automata method is detailed described in...
the papers [9–12]. Due to mobility of automata and the possibility of switching the connection state of the neighbors, it is possible to simulate also destruction of old and formation of new surfaces profiles.

2. Numerical model

The simulated setup is shown in Fig. 1a. The diameter of automata was equal to 2.5 nm. The top block of the setup imitates the moving body, whereas the bottom block the body in rest. The coordinates of automata of the bottom layer of the bottom block have been fixed. The elements of the top layer of the top block were forced to move along the \( x \)-axis with velocity \( V_x \) (the time dependence of \( V_x \) is depicted in Fig. 1b). In a normal direction (along the \( y \)-axis), the upper layer of automata was subjected to force \( F_y \), with time dependence as shown in Fig. 1c. In order to prevent the appearance of ‘impact’ effects connected with sharp changing of values of velocity or pressure, procedure of linear increasing of loading up to the certain value was used. For modeling an extended sample the periodic boundary conditions along the \( y \)-axis have been used.

Modeling of sliding friction in of contact area has been executed at various values of relative velocity of sliding and normal pressure (\( v = 2, 3, 4, 5 \) m/s, \( P = 125, 255 \) and 383 MPa which corresponds to 1/4, 1/2 \( \pi 3/4 \) of yield stress).

3. Sample parameters

The material parameters used in the simulations correspond to the rail steel [12]. Stress–strain diagram of such material is presented on the Fig. 2. The automata parameters corresponding to the properties of the simulated material are presented in Table 1. For transition of pair of interacting automata from a ‘linked’ state into a ‘unlinked’ state the criterion on the basis of calculation of stress intensity in the considered pair was used. This parameter was compared with the value of material strength; the criterion of transition can be written as:

\[
s_{ij}^{(l)} \geq K \sigma_{ij}^p,
\]

(2)

or

\[
s_{ji}^{(l)} \geq K \sigma_{ji}^p.
\]

(2a)

Fig. 1. Simulated setup and external loading conditions: (a) structure and parameters of the setup, loading scheme; (b) loading velocity profile; (c) loading pressure profile.

Fig. 2. Stress–strain diagram for rail steel.
Here $s_i^{(j)}$ is the strength of material of automaton $i$ or $j$ correspondingly, and $K^j$ is the coefficient characterizing cohesion properties between interacting materials. The value of parameter $s_i^{(j)}$ was calculated on the basis of theory of small elastoplastic deformations for planar stressed state and can be written as

$$s_{int}^{(j)} = \sqrt{(s_{ij}^x)^2 + (s_{ij}^y)^2 - s_{ij}^x s_{ij}^y + 3(t_{ij})^2},$$

(3)

here $s_{ij}^x$ and $s_{ij}^y$ are normal components of stresses in the given pair of automata $i$ and $j$, $t_{ij}$ are tangential components. In present paper, $K^j$ was equal to 1 that is all the interacting automata represent the same material.

For transition of pair of automata from unlinked state into linked state (welding), a similar criterion based on calculation of stress intensity was used. As stress intensity in the contacting pair have become larger than the corresponding value of material strength $s_i^{(j)}$, the pair of automata passed into a linked state.

4. Results of simulation

4.1. ‘Quasi-fluid’ layer formation

The friction of two elastoplastic bodies is accompanied by formation of strongly pronounced dynamic layer—a ‘quasi-fluid’ layer [6–8]. The processes occurring in it are plastic deformation deformation, degradation, formation of new bonds and intensive processes of mixing of particles of both surfaces. After running-in stage, the processes of destruction and restoration of continuity in the sliding layer come into a dynamic equilibrium. The typical structure of the sliding layer and structure of bonds between automata at steady-state stage are shown on Fig. 3a and b accordingly.

As it was noted in the sited papers, thickness of the ‘quasi-liquid’ layer is a function of normal pressure and relative sliding velocity. It can be seen in Fig. 3c and d, that at higher values of normal pressure an increase of thickness of the sliding layer is observed.

There are several aspects of the present simulations, which are of interest for problem of development of surface

![Fig. 3. Fragment of the simulated setup at steady-state regime of friction. (a) Structure at $F_y = 255$ MPa and $V_x = 3$ m/s; (b) net structure at $F_y = 255$ MPa and $V_x = 3$ m/s; (c) structure at $F_y = 383$ MPa and $V_x = 5$ m/s; (d) net structure at $F_y = 583$ MPa and $V_x = 5$ m/s.]

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### Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus</td>
<td>$E = 206$ GPa</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>$\mu = 0.3$</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho = 7800$ kg/m$^3$</td>
</tr>
<tr>
<td>Yield point</td>
<td>$\sigma_y = 510$ MPa</td>
</tr>
<tr>
<td>Strength</td>
<td>$\sigma_c = 920$ MPa</td>
</tr>
<tr>
<td>Ultimate strain</td>
<td>$\varepsilon_c = 0.12$</td>
</tr>
</tbody>
</table>
topography. As shown in the paper by Schargott and Popov (in this issue), development of the surface topography can be modeled as stochastic mass transport inside the friction zone. The two main kinds of elementary transport processes are: (i) transport along the surface and (ii) transport from and to the surface. These stochastic transport processes can be described as effective diffusion process in the lateral and vertical directions. To be able to apply the phenomenological theory by Schargott and Popov it is necessary to get the effective diffusion coefficients. The transport from and to the surface leads to the stochastic wandering of the average position of the quasi-fluid layer. Analysing this wandering can give the necessary information for the phenomenological theory of surface formation. The time dependence of the coordinate of the position of layer is depicted on Fig. 4. This value was estimated as average value of Y coordinates of all automata inside ‘quasi-liquid’ layer. Within the limits of time corresponding to eight cycles the position of quasi-fluid layer changes in stochastic manner. Regrettably, we still do not have sufficient statistics to estimate the effective diffusion coefficient from these data. This will be done of the basis of further simulations.

4.2. Surface topography analysis

As it was already mentioned above, capabilities of movable cellular automata method allow one to simulate directly destruction of existing bonds between particles and formation of new places of couplings. Thus it is possible to lead the analysis of topography of generated surfaces. To this end a curve describing all bonds, connected with one of contacting surfaces has been constructed. Such ‘surface profile’ for the bottom surface is shown in Fig. 5. We then made discrete Fourier transform of this surface profile. The scheme of digitization of the received function \( f \) is represented in Fig. 6. The size of step of digitization corresponds to radius of the automaton (the minimal distance between centers of two automata located one above the other in a close package). It corresponds to size of the minimal ‘asperities’ on the considered surface. The power spectrum of the surface can be written as

\[
c^2(K_n) = a^2(K_n) + b^2(K_n),
\]

where \( K_n = 2\pi n/l, \ n — \text{integer and } n \in (0, ..., M), \ M = \delta/l \) with Fourier coefficients \( a(K_n) \) and \( b(K_n) \) defined as:

\[
a(K_n) = \frac{2}{l} \int_0^l f(x) \sin(K_n x) dx = \frac{2}{l} \sum_{m=1}^M f_m \left( m \cdot \frac{\sin(K_n x)}{(m-1)\delta x} \right)
\]

\[
b(K_n) = \frac{2}{l} \int_0^l f(x) \cos(K_n x) dx = \frac{2}{l} \sum_{m=1}^M f_m \left( m \cdot \frac{\cos(K_n x)}{(m-1)\delta x} \right)
\]

\[(5)\]

After calculating the integrals:

\[
a(K_n) = \frac{2}{l} \sum_{m=1}^M f_m \left( -\frac{1}{K_n} \cos(K_n x) (m \cdot \frac{\sin(K_n x)}{(m-1)\delta x}) \right)
\]

\[
b(K_n) = \frac{2}{l} \sum_{m=1}^M f_m \left( \frac{1}{K_n} \sin(K_n x) (m \cdot \frac{\cos(K_n x)}{(m-1)\delta x}) \right)
\]

\[(6)\]

In Fig. 7 the curves describing structures of top and bottom surfaces for the case \( V_c = 3 \text{ m/s} \) and \( F_n = 255 \text{ MPa} \), in axes \( \log(c^2) \) and \( \log(K_n) \) are presented. The value for \( \log(c^2) \) were averaged on five structures during various time.
moments. The power spectra show a typical for fractal surfaces dependence on the wave vector with the slope ‘−2’.

Similar dependence have been constructed for other values of relative sliding velocity and pressure. Curves for the bottom surfaces for pressures $F_y = 255$ MPa and $F_y = 127$ MPa at $V_x = 2$ m/s are represented in Fig. 8a and $V_x = 5$ m/s in Fig. 8b. It is easily seen, that in both cases the curves describing power spectra at higher pressure are located above the curves corresponding to a lower pressure $F_y = 127$ MPa. It means, that larger pressure leads to a formation of more rough surface. At the same time, with increasing the $V_x$ this difference decreases.

5. Conclusions

The following general conclusions can be drawn from our results:

- Formation of quasi-liquid layer and its random migration during friction has been shown.
- The power spectra of running in surfaces show a typical for fractal surfaces dependence on the wave vector with a slope ‘−2’.
- It was shown, that roughness parameters of surface dependent on external pressure. Increasing of pressure leads to increasing of roughness.

Fig. 7. Power spectra for surface profiles at $F_y = 255$ MPa and $V_x = 3$ m/s.

Fig. 8. Power spectra for surface profiles at $F_y = 255$ MPa and $F_y = 127$ MPa: (a) $V_x = 2$ m/s; (b) $V_x = 5$ m/s.
6. Uncited reference

[13].

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References