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Computer simulation of precision contact with account of microgeometrical and mechanical heterogeneity of surfaces

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Abstract

Computer model of 3D contact based on SPM research of contact surfaces is offered. The main idealizing model feature is linear character and additivity of material deformation on separate contact sites of 3D-images. The model takes into account multilevel topography of surfaces, map of elastic properties of materials, superficial forces effect and non-uniformity of intercontact gap. The map of elastic properties of materials was obtained from the SPM phase contrast images. It is shown, that heterogeneity of micromechanical properties of materials in the contact zone results in essential redistribution of contact spots, contact stresses and adhesive forces. Statistical peculiarities of contact formation depending on probability of mutual collisions of rough surface sites are considered, including during sliding. The efficiency of offered computer model to describe precision contact including multilevel one is considered using examples of interaction between worn TiN coating.

Keywords: Atomic force microscopy; 3D topography; Phase imaging; Micromechanical heterogeneity; Real contact area simulation; TiN coating

1. Introduction

Study of a precision contact is now an actual task due to current trends in miniaturization of moving joints in precision mechanics, computer engineering, optics, electronics, medical engineering, etc. The works are inspired also by activity in the field of microelectromechanical systems (MEMS) that are characterized by the functional elements of micrometer size [1].

Creation of new precision friction assemblies demands development of new experimental methods to estimate topography parameters of smooth surfaces, to elaborate their contact models and techniques for evaluation of their workability at friction.

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Contact of smooth surfaces separated by nanometer gap features formation and operation under joint action of geometric (size and shape of asperities), mechanical (deformation of the material, formation and break of frictional links) and physical (superficial and capillary forces) factors. No one of these factors can be neglected when studying the precision joint and their contributions are significantly nonadditive.

One more factor that is important for the analysis of a precision joint is heterogeneity of micromechanical properties of materials in surface layers. That results from their structure, discontinuity of boundary layers and presence of coatings.

The aim of the work is to give a more adequate description of a precision contact formation using computer 3-D simulation of the surfaces' contact interaction with account of their geometric (topography) and micromechanical heterogeneity.

2. Experimental study

Scanning probe microscopy currently provides the most effective method for obtaining all the data sets necessary for calculation of a precision contact. A combination of different modes of scanning and force spectroscopy [2] allows one to obtain quantitative information on the surface topography and adhesion activity as well as on the micromechanical properties of the material superficial layers (Fig. 1).

Two scanning modes can be employed for estimation of the micromechanical properties of the superficial layers—contact mode and tapping mode. They both feature direct contact of the probe tip with the sample. Under the contact mode, the tip is in constant touch with the surface and we obtain a map of the tip friction against the surface. It is in complex connection with contact properties of the surface. However, contact mode enables measurement of force vs. distance curves that can then be used for estimation of elastic modulus and surface energy of the tested material.

The tapping mode is characterized by short-time contact of the tip and the surface. It provides

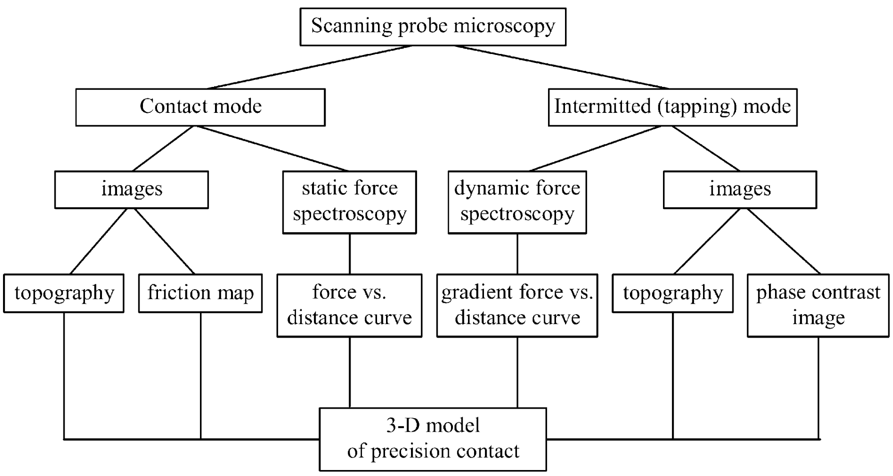

Fig. 1. SPM modes for preparation of initial data for computer simulation of precision contact.

the reverse possibility of high-resolution mapping of the heterogeneity of micromechanical properties on phase contrast images that describe the material's local hardness. But quantitative interpretation of the measured data is still quite complex even with the help of dynamic force distance curves.

In the proposed approach to calculation of a precision contact, we used the latter mode. However, it demanded interpretation of the material properties by an expert.

SPM measurements were done with experimental system NANOTOP-203, developed in the laboratory of surface micromechanics of MPRI NASB. The instrument used a tungsten probe and detection system based on an optic-fiber interferometer. Working resonant frequency of the probes was 45 to 60 kHz.

At scanning under the tapping mode, surface sites with different micromechanical properties shift the probe cantilever oscillation phase in different ways. The magnitude of the phase shift ϕ was recorded in an additional phase image file along with a file of the probe Z-position describing the surface topography over the studied site. A feedback system provided constant probe oscillation amplitude.

It was shown that the magnitude of the phase shift depends on the material stiffness in the scanned point [3]:

$$\phi_j \approx \frac{Q\sigma_j}{k},$$

where Q is the probe quality factor; $\sigma_j=\Sigma_i \partial F_i/\partial z$ is a sum gradient of forces influencing the probe tip, in the case of elastic interaction between tip and sample it can be interpreted as material local hardness; k is the cantilever stiffness constant.

For the computer simulation it is convenient to use a specific stiffness $\sigma_j^*=\sigma_j/S_j$ where S_j is area of contact of tip and surface. Assuming the contact area is governed by Hertzian law and the load on the tip is defined by the cantilever bending, we can obtain a dependence describing the phase shift as a function of the material local elastic modulus and parameters of the measurement system [4]:

$$\sigma_j^* \approx \frac{3 \qquad k\phi^2}{2\pi R Q^2 A_0(1-r_{sp})},$$

where R is the tip curvature radius (about 100 nm); A_0 is an amplitude of the probe free oscillation; $r_{sp}=A_{sp}/A_0$ is a set-point parameter; A_{sp} is an amplitude of probe cantilever oscillation at the scanning that is kept constant.

The probes were made by electrochemical etching and their stiffness was 300–800 N/m that exceeded significantly stiffness of commercial probes. That allowed us to obtain the phase contrast images for hard materials. As an example, let's consider the surface of a TiN coating which has been subjected to friction against a steel roller.

3. Computer model of a precision contact

Precise computer representation of the surface topography is available due to height function $Z(x, y)$. For the considered site, it is numerically described by the SPM image matrix.

Computer simulation was conducted for the site of a rough elastic surface with the relief height $z_j=Z(x_j,y_j)$ measured in the nodes of scanning net, that contacted with smooth rigid plane. Force of resisting to deformation for elementary column of the material at point j is a function of approach σ_j (model of Winkler layer) [5] (Fig. 2)

$$P_j=\sigma_j^* \Delta x \Delta y \delta_j. \tag{3}$$

Molecular interaction of the surfaces is characterized by Lennard–Jones potential. Shape of the deformed surface is defined by the material compression dz_j in the areas of contact and non-contact tension beyond them. Direction of the resultant force over elementary area $\Delta x \Delta y$ on the image was determined from the force balance. It enabled visualization reflecting real contact area A_r.

For a new surface $z_j'=z_j+dz_j$, after summation over corresponding image nodes we calculated nominal contact stress p and non-contact adhesion force between the surfaces F_s. They were found from corresponding deformation levels h as

$$p(h)=-\Delta x \Delta y \sum_j \sigma_j^*(h-z_j'); \tag{4}$$

$$F_s(h)=\frac{8}{3}\varepsilon^2 \Delta x \Delta y \sum_j \Delta\gamma_j (h-z_j')^{-3}, \tag{5}$$

where ε is an interatomic distance for the studied material; $\Delta\gamma$ is specific surface energy. Resultant force between contact and non-contact forces is not equal to zero for the considered surface site and depending on the sign corresponds to either external compressive force or adhesion when the surfaces are separated.

So, the algorithm of calculation comprises the following stages:

1. obtaining Z- and ϕ-images;
2. building σ- and $\Delta\gamma$-images;
3. calculation of function $p(h)$ with its visualization and determination of parameter h;
4. calculation of F_s, A_r and their visualization.

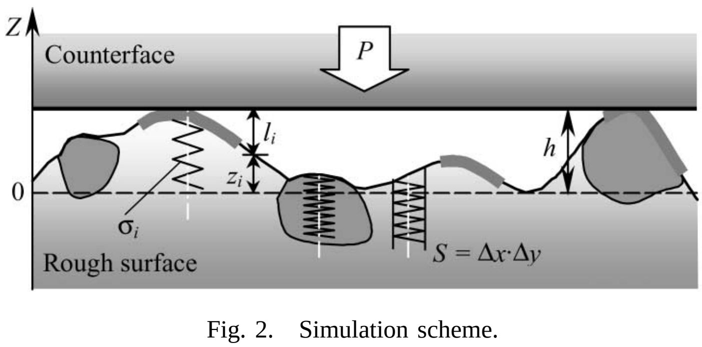

Fig. 2. Simulation scheme.

4. Results of investigation

Figure 3 shows the initial topography (*a*) and phase contrast (*b*) images for worn TiN coating [6] for scan 18×18 μm. Figure 3c shows a mixed image of the TiN coating surface that was

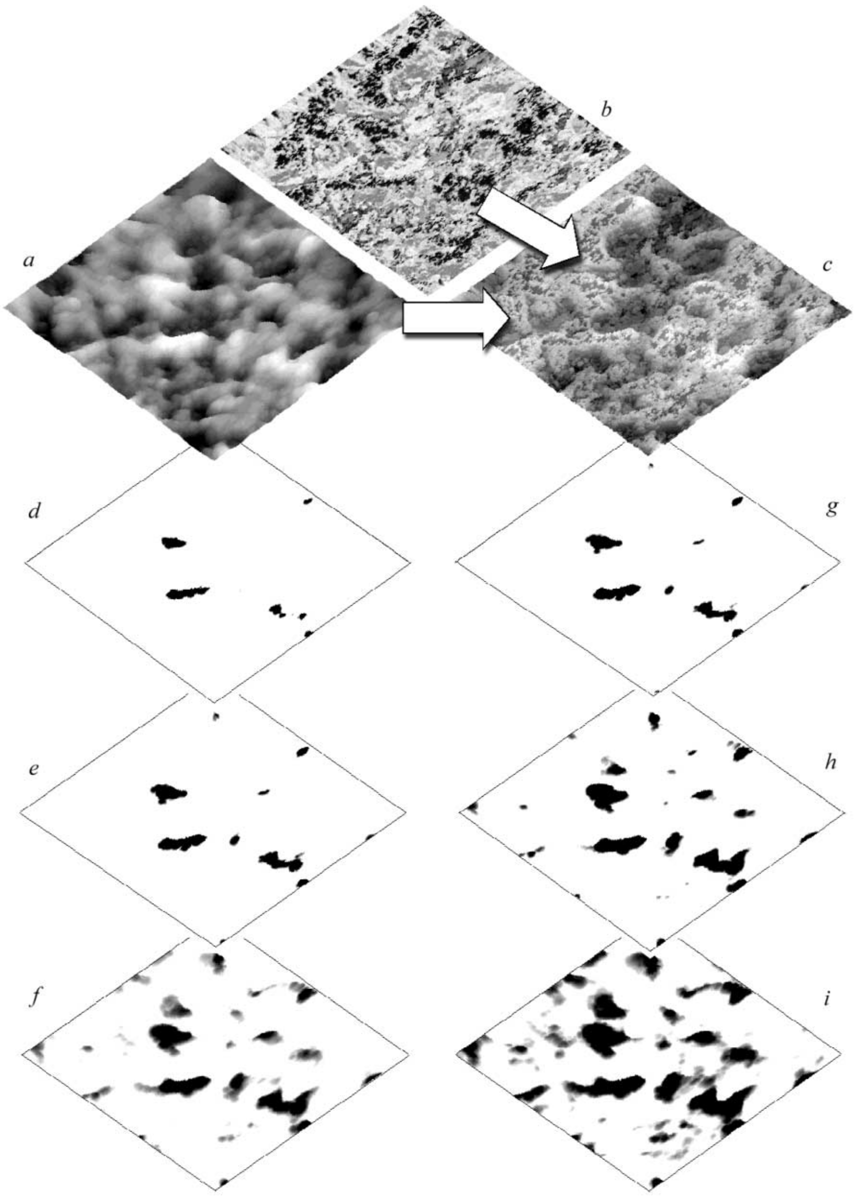

Fig. 3. Computer simulation of contact for TiN coating (a) without (d, e, f) and with (g, h, i) account of microgeometrical and micromechanical heterogeneity of the surface. (a) Topography image. (b) A phase contrast image. (c) Mixed image obtained by overlaying images (a) and (b). (d) and (g) Contact pressure distribution under load 264 MPa. (e) and (h) Contact pressure distribution under load 645 MPa. (f) and (i) Contact pressure distribution under load 5570 MPa.

obtained by overlaying the topography and phase images. Dark spots on the asperities' tops correspond to areas of thin tribolayers (thickness 2–4 nm). On the slopes, areas of material having less hardness than TiN were observed. These sites correspond to areas of plastic smearing of material of the steel roller.

Real contact area and molecular interaction force (adhesion and real contact pressure) of the surfaces as a function of load was calculated according to the above algorithm. Results of visualization of the contact zone are given in Figs. d–f and g–i. It is seen that taking into account micromechanical heterogeneity of the material surface, we can significantly correct estimations of the contact performances. With load growth, asymmetry in formation of areas of real contact becomes more noticeable. It can be conditioned by involving softer transferred layers into the deformation.

To estimate the effect of material heterogeneity on the contact characteristics, we can analyze the ratio between the values of A_r and F_s calculated for the different assumptions of the simulation (Fig. 4). The assumption of a heterogeneous worn TiN coating gives greater values for the real contact area and molecular adhesion force between the surfaces compared with the simulation results for the coating with homogeneous properties.

However, the influence of the transferred layers is not the same under different pressures on the rough surface. Soft and very thin tribolayers on the tops of asperities under low loads increase molecular adhesion force between the surfaces rather than change the contact spot areas. Transferred layers of steel that are softer than TiN are deformed under certain contact pressures and provide an additional increase in the real contact area and molecular adhesion force of the surfaces (extreme points on curves 1 and 2, Fig. 4).

5. Conclusion

A 3-D computer simulation is possible with the use of a set of SPM images obtained under the tapping mode and describing topography and micromechanical heterogeneity of the studied surfaces. Quantitative characterization of maps of the surface properties is possible due to the participation of an expert. Additional procedures of nanoindentation and force spectroscopy over

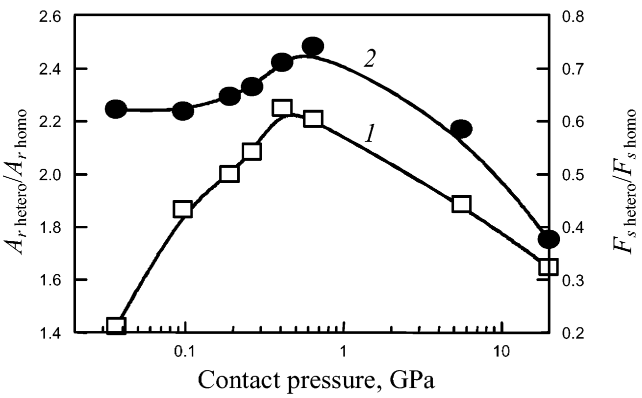

Fig. 4. Ratio $A_{r\ \mathrm{hetero}}/A_{r\ \mathrm{homo}}$ (1) and $F_{s\ \mathrm{hetero}}/F_{s\ \mathrm{homo}}$ (2) as function of contact pressure.

the studied surface site can help to improve the objectivity of the initial data preparation for the calculation. The model adequacy can also be improved by distinguishing and taking into account bulk heterogeneity of the material as well as heterogeneity in thickness of the surface films.

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