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MODELLING OF CONTACT OF STRUCTURED MATERIALS BASED ON DATA FROM SCANNING PROBE MICROSCOPY

Sergey A.Chizhik*, Zygmunt Rymuza**, Dmitri I. Shasholko***

*Institute of Heat and Mass Transfer of the Academy of Sciences of Belarus, Minsk, Belarus

** Warsaw Uniersity of Technology Institute of Micromechanics and Photonics, Warsaw, Poland

*** MicrotestMachines Co., Gomel, Belarus

Summary Foundations of mechanical characterisation of structure and local elastic modulus for nanocomposites using scanning probe microscopy have been considered. Proposed were schemes to obtain input data for 3D modelling of contact of heterogeneous materials. They provide for imaging topography and mapping of structure and local micromechanical properties. Algorithms for computer modelling of contact of micro- and nanostructured composites have been described.

Introduction

Development of composites with fine micro- and nanostructure and their application in precision joints and microelectromechanical systems (MEMS) require an adequate description of the contact [1-4]. Difficulties in modelling of the contact of structured materials are conditioned by the necessity to consider heterogeneity of surface geometry (roughness, difference of film thickness) and physico-mechanical properties (elastic modulus, surface free energy) of the material surface layers.

New possibilities, however, appear with application of research methods employing scanning probe microscopy (SPM), particularly atomic force microscopy (AFM). Imaging in SPM is attributed by contact interaction between the probe tip and the sample material and results in static and dynamic phenomena in the probe cantilever [2, 3].

Input data preparation

AFM measuring system traces the probe cantilever movements and builds images based on these data. The measured data contain also information about the probe tip interaction with the tested sample surface. Heterogeneity of the material elastic properties caused by material structure and presence of different components can be mapped in contrast images. We analyzed micromechanical aspects of the AFM image formation and their relationships with local mechanical properties of materials. The analysis showed that the cantilever oscillation phase shift near the researched surface correlates with local elastic modulus of the material. That allows mapping of the physico-mechanical heterogeneity of surfaces. Proposed were the solutions of the contact problems that consider influence of surface forces and material layered structure (Fig. 1).

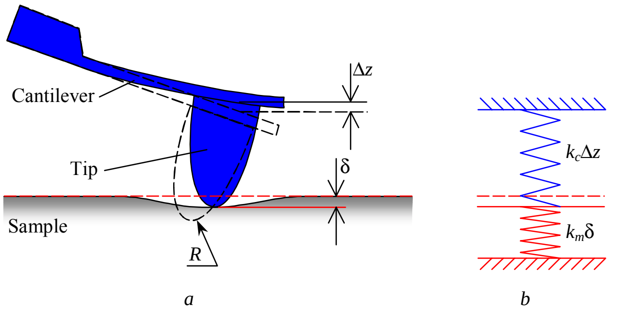


Fig. 1. Schematic diagram of the interaction between probe and sample surface (a) and mechanical model of the tip-sample interaction (b)

The experimental functions of interactions between the tip and the tested material were based on data obtained by analysis of force-vs-distance curves (static force spectroscopy) and dependencies of force gradient (oscillation amplitude) on tip-to-sample distance. We proposed algorithms for evaluation of the local elastic modulus and surface free energy and described the formation of the calibrated maps of the distribution of physico-mechanical properties over the surface. Result of the input data preparation is an equivalent topography image and map of reduced elastic modulus that are used then in the contact modelling. We discuss also the possibilities of surface nanotomography that is based on the phenomenon of non-uniform deformation of the surface layer by the tip with when harder inclusions are present in soft matrix. That allows obtaining information about heterogeneity of the material across its depth.

Contact zone modelling

As the result of the complex applications of the SPM methodology we propose to use the set of topography images, maps of the elastic modulus and surface free energy as input data for modelling contact of two rough surfaces.

We also tried to elaborate the spatial model of the real contact area for the structured materials with the application of the results of experimental studies.

In an elastic contact, the pressure and deformation of all surrounding points in the contact affect the displacement of a point under the load. The relationship is simplified in the Winkler surface model or elastic foundation model, where the contact surface is modelled as a set of elastic bars. The shear between them is neglected, so the contact pressure at a point is only dependent on the actual deformation at the point. The elements are considered as linear elastic bars of length h_d and with a spring constant or stiffness σ_j in z direction. Physical sense of h_d is the deformed layer depth. Resisting force against deformation for an elementary bar of material at point j is a function of approach δ_j (model of Winkler layer)

$$P_j = \sigma_j \,\Delta x \Delta y \delta_j. \tag{1}$$

Local effective stiffness σ_j is calculated at every data point from equivalent local elasticity modulus

$$E = [(1 - \nu_1^2)/E_1 + (1 - \nu_2^2)/E_2]^{-1}, \tag{2}$$

where ν_i, E_i (i=1,2) is the Poisson ratios and elastic moduli of the contacting materials respectively.

Molecular interaction between two surfaces is characterized by Lennard–Jones potential. The shape of the deformed surface is defined by the material compression dz_j in the areas of contact and non-contact tension beyond them [10]

$$dz_j = \frac{8}{3} \Delta\gamma h_d \varepsilon^2 E_j^{-1} l_j^{-3} dz_j \,, \tag{3}$$

where l_j – is a local gap between the contacting surfaces.

The direction of the resultant force over elementary area $\Delta x \Delta y$ in the image was determined from the force balance. It enabled visualization of reflecting real contact area A_r.

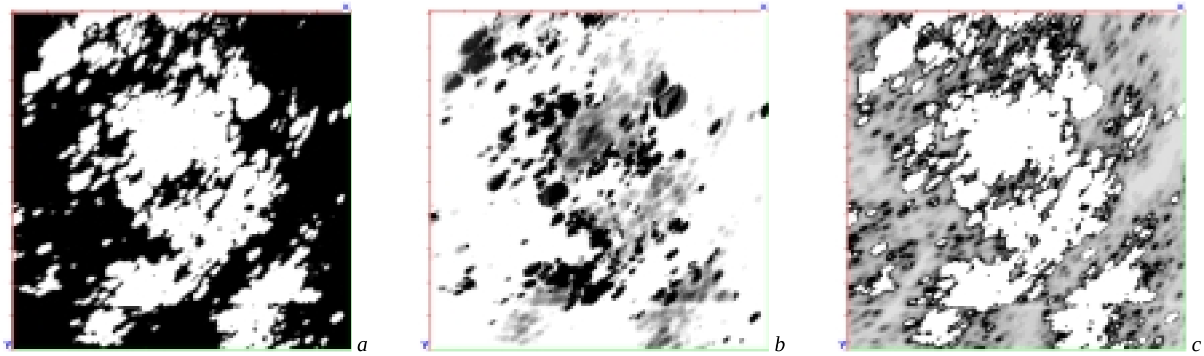
For a new surface $z_j' = z_j + dz_j$, after summation over corresponding image nodes we calculated nominal contact load P and non-contact attractive molecular force between the surfaces F_s. They were found from corresponding deformation level h as

$$P(h) = -\Delta x \Delta y \sum_j \sigma_j \left(h - z'_j\right); \tag{4}$$

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

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

Figure 2 shows results of the contact interaction simulation between two rough DLC surfaces.



a *b* *c*

Fig. 2. Visualized results of simulation of contact between two rough DLC surfaces: a – real contact area, b – distribution of contact pressure, c – molecular adhesive forces between the surfaces

Conclusions

A complex approach to characterization of the contacting surfaces with help of AFM and including measurement of topography, evaluation of heterogeneity of micromechanical properties and their quantitative characterization provides information for modelling the contact interaction of heterogeneous materials. Preparation of the input data and modelling of the precision contact can be realized using specialized atomic force microscope NT-206 and SPM processing software SurfaceView.

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