# Modeling of contact interaction between atomic force microscope probe and an elastic brittle damage material

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**Abstract**

Atomic force microscope (AFM) can be used to obtain information not only about the topology of the internal structure of the material, but also on its local physical properties. The corresponding theoretical models must be used for correct decoding of the experimental results. Modeling the contact interaction of AFM probe with the elastic brittle specimen is presented in this paper.

At this stage of the research it was considered that the mechanical behavior of a model sample is described by Neo-Hookean elastic potential. Mechanical strength of the reaction to the probe indentation was determined from the solution of the corresponding contact boundary problem. The required solution sought numerically - the finite element method (in nonlinear elastic axisymmetric formulation) was applied used. As a result, we obtained dependencies of the mechanical response force on the depth of indentation, specimen elastic modulus and geometric characteristics of the probe: the radius of the top and cone angle.

Processes of AFM probe cyclic indentation into fragile medium damaged by deformation were numerically investigated using this approach. AFM probe pressed repeatedly in the same place on the sample surface, that improves the accuracy of measurements. Theoretical modeling is to aid in its adequate decryption.

As a result, the dependencies of reaction force on the probe depth of penetration and the size of the hole formed after the previous contact. Probe indentation into the surface with the existing microwells, which simulated caries damaged tooth is also modeled.

Atomic force microscopy (AFM) is one of the most promising research tools for nanoscale materials level. They can be used to obtain information not only about the topology of the internal structure of the material, but also on its local physical properties [1, 2, 3, 4]. You can get unique information about the mechanical properties of materials at the nanoscopic level, exploring the process of introducing the probe into the specimen: the emergence of dislocations, the occurrence of shear instability, phase transitions and many other phenomena that are inaccessible to the previously known techniques [5]. The corresponding theoretical models (which contain additional knowledge about the subject of study) must be used for the correct interpretation of the experimental results [6, 7, 8]. One such approach modeling the contact interaction between the AFM probe and the sample surface is presented in this paper.

Design model scheme consists of a specimen with a flat surface (investigated material) and an indenter (AFM probe) in the form of a cone with a rounded apex (Fig. 1). The surface may contain different types of wells.

It is considered that the probe is absolutely rigid, and mechanical behavior of a model sample can be described by the Neo-Hookean elastic potential. The mechanical force of the reaction to the probe indentation is determined from the solution of the corresponding

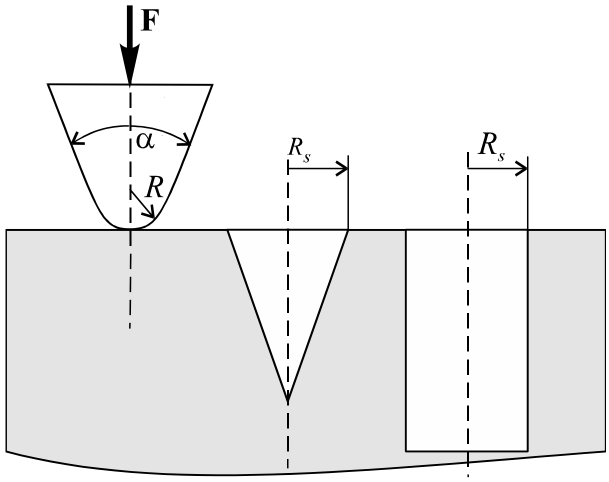


Figure 1: Design scheme of contact interaction of the AFM probe with the specimen

contact boundary-value problem. The required solution sought numerically - using the finite element method (in the nonlinear elastic axisymmetric formulation). As a result, we obtain the dependence of the elastic reaction force on mechanical properties of the specimen material and geometric characteristics of a probe tip radius $R$ and the cone angle $\alpha$.

Comparison of the nonlinear solution (in the case of finite nonlinear elastic deformation) with the known problem of the Hertz contact of two linear-elastic spheres under small deformations was carried out using this model [9]. At present this solution is widely used in practice for the first assessment calculations. It is a standard set of software most of the AFM. Hertz's formula for the case when one of the spheres has an infinitely large radius (i.e. contact with the half-plane) and the second is absolutely rigid has the following form

$$F_{Hertz} = \frac{4E_s R^{1/2}}{3(1-\nu_s^2)} u^{3/2} \tag{1}$$

where $E_s$ — the initial Young's modulus of the specimen, $\nu_s$ — Poisson's ratio (all hereinafter: the index "$s$" means that the parameter refers to the sample). For the case of nonlinear elastic contact problem similar dependence has the form

$$F = 8.6 C_s R^2 \left(\frac{u}{R}\right)^{1.3} \tag{2}$$

where $C_s$ — Neo-Hookean elastic constant. For an incompressible medium $\nu_s = 0.5$, then $C_s$ corresponds to the initial Young's modulus as $E_s = 6C_s$. Fig. 2 shows the dependence of reaction force $F$, acting on the tip on the depth of its penetration into the material $u$, calculated from Hertz formula and numerically (Neo-Hooke). The graphs show that the divergence of Hertz formula and non-linear elastic solution starts at $u/R > 0.4$ (and non-linear elastic solution gives higher values of force). For smaller values it is quite possible to use Hertz formula.

Different types of probes are used, depending on the mechanical properties of tested on the ACM materials. In the study of elastomers and soft thermoplastics probes with a smaller cone are usually used, for relatively hard samples, respectively, more "blunt"

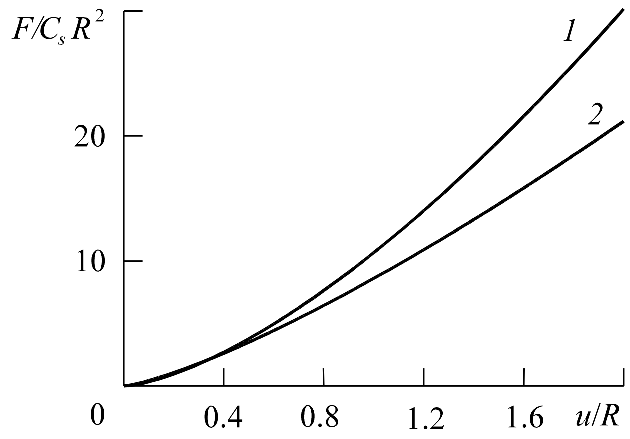


Figure 2: Dependences of reaction force $F$, acting on the tip, on the depth of its penetration into the material $u$. 1 — Hertz formula, 2 — numerical nonlinear elastic solution (Neo-Hooke)

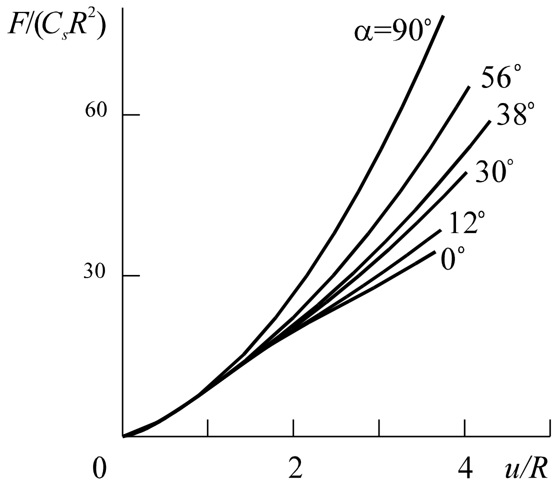


Figure 3: Dependence of reaction force $F$ on AFM probe penetration depth into the specimen $u$ and cone angle $\alpha$

(and stronger) indenters are chosen. In determining the dependence of $F$ on $\alpha$ values of the arguments ranged from 0 (cylindrical probe with a rounded apex of radius $R$) to 90° (Fig. 3).

Calculations show that the angle of the probe cone begins to significantly affect the reaction force when the depth of penetration of the probe into the specimen reaches values of $3 - 4R$, that is, this factor should be necessarily taken into account in describing large deformation in the contact zone. Thus, when the indentation of the probe to a depth of $4R$, $F(\alpha = 90°)$ more than twice the $F(\alpha = 0°)$.

The problem of repeated indentation of a hard "blunt" AFM probe (($\alpha = 90°$) in a brittle breaking in the process of deformation elastic material has been solved using this approach. The corresponding model studies carried out.

Repeated indentation of the AFM probe into the same place of damageable elastic brittle surface was modeled, and after each contact in the sample had ever increasing hole depth $\delta$. Hole is a result of brittle fracture of the material during the probe indentation, that is, changing the geometry the specimen surface happens but without residual plastic

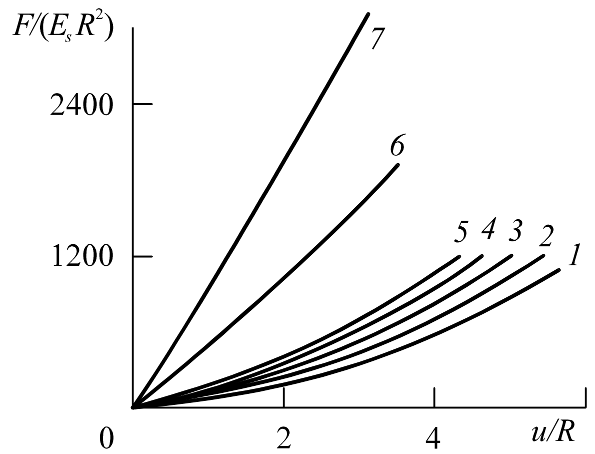


Figure 4: Dependence of reaction force $F$ on AFM probe on the depth of its indentation $u$ into brittle sample and depth of the hole $\delta$: $1 - \delta/R = 0$, $2 - 0.5$, $3 - 1$, $4 - 1.5$, $5 - 2$, $6 - 5$, $7 - 10$

stresses. Such processes are characteristic, for example, for AFM studies of tooth enamel. The enamel can have different mechanical properties of its thickness(a variety of injuries can be on the surface, the surface can be covered with a thin coating of another material, etc.). Repeated indentation into the same place of tooth enamel can help to gather the necessary information about its true mechanical properties, and mathematical simulation of this process should help in deciphering the data adequately.

As a result, dependences of the reaction forces on depth of probe indentation and the magnitude of the hole formed after the previous contacts were built (Fig. 4). The movement of the probe into the material after the occurrence of contact between it and the bottom of the hole was taken as $u$. It was established, the deeper the hole, the greater the effort required for its further growth. At very large depths (curves 6 and 7) dependence of $F$ on $u$ were practically linear, and they were lying significantly higher than the other curves.

The surface of a tooth can not always be regarded as flat and smooth. Therefore, the task of impressing a hard indenter into conical and cylindrical holes in brittle elastic surface has been solved (see Fig. 1). These grooves simulated caries microdamages in tooth enamel. Dependences of the force pressing the AFM probe $F$ on the depth of penetration of $u$ into a conical cavity with radius $R_s$, when the indenter has the form of a cone ($\alpha = 90°$) with rounded apex radius $R$ are shown in Fig. 5. Angle of the cone-shaped hole $\alpha_s$ was 70° (solid lines) and 90°90 (dashed lines). Variants when the probe tip radius was equal to the radius of the hole, or exceeded it in 1.5, 2, 3 and 4 times were calculated. The calculations show that the value of $F$ is weakly dependent on the relation between $R$ and $R_s$. The graphs are the limiting curves for the cases of $R/R_s = 4$ and $R/Rs = 1$. Rest dependencies lay between them. For wells with a gently sloping sides ($\alpha = 90°$) curves were slightly higher (but insignificant).

Also, a similar problem on a conical indentation of the AFM probe in a cylindrical cavity of radius $R_s$ (the limiting case of “degeneracy” cone-shaped hole in the cylinder) for different values of probe cone angle $\alpha$ has been solved. $\alpha$ was taken to be 40°, 60°, and 90°. The results are shown in Fig. 6. The curves corresponding to $\alpha = 90°$, also lay close to those shown in Fig. 5, so a form of wells not very effect on strength of the reaction (for the considered range of $\alpha_s$ values). A different situation is observed for the parameter $\alpha$. As can be seen from the graphs in Fig. 6 the reaction force of the probe indentation into the cavity depends strongly on the “sharpness” of the cone. The larger $\alpha$, the harder it is

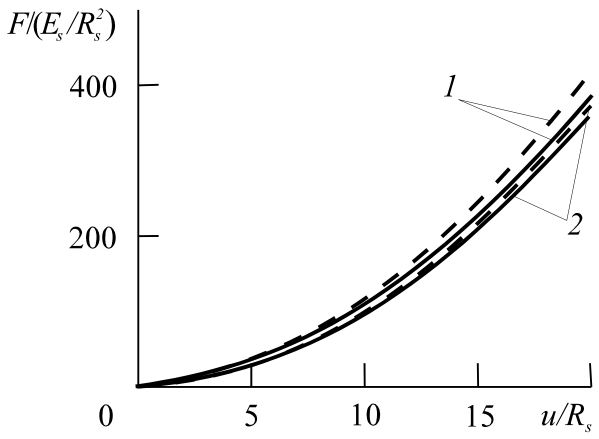


Figure 5: Indentation the conical probe (full cone angle $\alpha = 90°$) with rounded apex of radius R in a conical cavity. Solid lines — $\alpha_s = 70°$. Dashed lines — $\alpha_s = 90°$. 1 — $R/R_s = 4$, 2 — $R/R_s = 1$

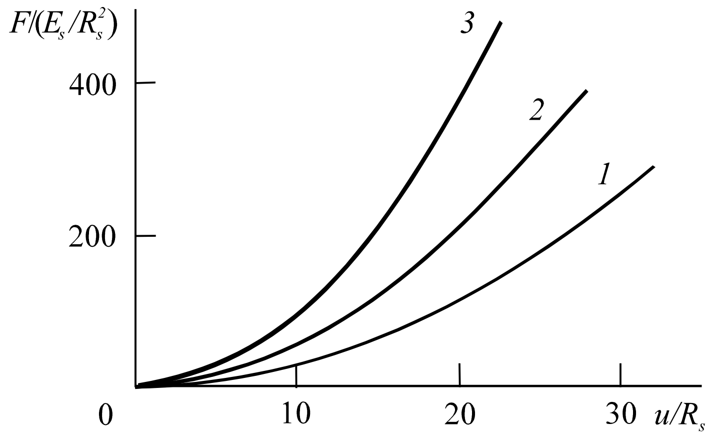


Figure 6: The indentation of a conical probe in a cylindrical cavity of radius $R_s$. 1 — $\alpha = 40°$, 2 — 60°, 3 — 90°

to enter the probe into the hole on the sample surface.

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