2.1. Cantilever

2.1.1 The Hooke's law

The cantilever is the most common sensor of the force interaction in atomic force microscopy. The atomic force microscope acquires any information about a surface because of the cantilever beam mechanical deflections which are detected by an optical system. In noncontact microscopy, resonators of the tuning fork-type are frequently used. Such sensors require tracking of the resonance frequency shift upon the probe-surface interaction onset.

Normally, cantilever is a beam in the form of a rectangular parallepiped (Fig. 1a) having length l, thickness t ($t \ll l$) and width w ($w \ll l$) or in the form of two beams connected at an angle (Fig. 1b) having a tip with length l_{tip} at its free end. Let us examine below the rectangular cantilever in detail. Its characteristic dimensions are shown in Fig. 1a. The probe's tip interacts with the surface. Assume that the point force acting from the sample is applied to the tip's apex.

The force acting on the probe has sometimes not only vertical but also horizontal components. Therefore, the cantilever tip can deflect not only along the Oz-axis but in two other directions: Ox and Oy (see Fig. 1a). Let's call the force vertical component F_z the normal force and longitudinal F_x and transverse F_y components — the lateral forces.

Because in AFM the tip-sample interaction influences the cantilever deformation, to determine the force one should know the cantilever deformation stiffness in various directions. Consider that the tip deflection vector $\mathbf{\Delta}$ (having components Δx , Δy , Δz) is linearly dependent on the applied force **F** in accordance with the Hooke's law [1]:

$$\mathbf{\Delta} = \mathbf{C}^{-1} \mathbf{F} \,. \tag{1}$$

The «constant» of proportionality is the second rank tensor C which we call the inverse stiffness tensor. It contains all the information about elastic properties of the cantilever.

To find the components of the tensor C it is necessary to solve the problem of the cantilever static deformation under the influence of forces directed along different axes. For the sake of clarity, we write the formula (1) as a matrix expression:

$$\begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix} = \begin{pmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{pmatrix} \begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}.$$
 (2)

Notice that the optical system detects not tip deflection but inclination of the cantilever top surface near its free end. Two angles are measured: deflection of the normal from vertical in the *Oyz* plane (angle α) and in the orthogonal direction – in the plane *Oxz* (angle β).

Instead of (2), we can write for the mathematical convenience the matrix expression relating angles α and β directly with force **F** components..

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} b_{\alpha x} & b_{\alpha y} & b_{\alpha z} \\ b_{\beta x} & b_{\beta y} & b_{\beta z} \end{pmatrix} \begin{pmatrix} F_{x} \\ F_{y} \\ F_{z} \end{pmatrix}$$
(3)

The introduced matrix, however, does not contain full information about the cantilever elastic properties in contrast to tensor C.



Fig. 1a. Rectangular cantilever with a tip.

Fig. 1b. V-shaped cantilever with a tip

- 1. The information about a sample in AFM can be obtained only from the cantilever deformation. The optical system allows to measure two angles defining the cantilever top plane inclination.
- 2. To determine the force acting on the cantilever one should know its elastic properties which are described by the second rank tensor of the cantilever inverse stiffness.
- 3. The deformation-force relation is modeled by the linear Hooke's law written as the tensor expression.

2.1.2 Deflections under the vertical (normal) force component (F_z)

Let us determine the magnitude and direction of the deformation arising from the vertical force F_z . Solution to this problem will allow to find components of the third column of tensor C (2).

$$\Delta x = c_{xz} F_z \,, \tag{4}$$

$$\Delta y = c_{yz} F_z, \tag{5}$$

$$\Delta z = c_{zz} F_z \,. \tag{6}$$

Deformation that we call here the vertical bending is shown in Fig. 2.



Fig. 2. Vertical deflection of the *z*-type

Next, let's examine a section of the beam. We will cut the beam and consider the deformation of the beam element having length L between the two cross sections (Fig. 3). Since this element is bent, the material at the outer edge is stretched in tension while at the inner edge it is compressed. Hence, there is a neutral plane of zero stress between the two surfaces. For calculations simplification we assume that the beam cross-sections remain planar and normal to their centroidal axis (pure bending of the uniform cross-section beam). This assumption is valid if $l/t \ge 8$ [2] which is true in our case.



Fig. 3a. Section of the bent beam

Fig. 3b. Beam cross-section

At the pure bending the neutral plane passes through the centroid of the beam cross-sectional area [3], i.e. in our case the parallepiped long axis belongs to the neutral plane. The material longitudinal extension ΔL is proportional to the distance z from the neutral plane: $\Delta L/L = z/R$ (see Fig. 2). According to the Hooke's law, the force acting on a unit area in a small strip near z with square dS is equal to dF = EzdS/R where E — Young's modulus, R — beam curvature radius. If any cross-section is considered, the forces are acting in one direction over the neutral surface and in the other direction below it. This makes a couple of forces producing the bending moment M_z which is a moment of forces with respect to the neutral axis:

$$M_z = \int_{S} z dF = \frac{E}{R} J_z .$$
⁽⁷⁾

The quantity J_z is called the axial moment of inertia of the beam section about the axis that passes through its centroid. For the beam with rectangular cross-section it is given by:

$$J_{z} = \int_{S} z^{2} dS = \frac{wt^{3}}{12}.$$
 (8)

By u(y) we denote the deflection of the beam point at the distance y from the fixed end in the z-direction. The curvature of the u(y) curve at small bends $(du/dy \ll 1)$ is given by $1/R(y) = d^2u/dy^2$. Then, taking into account expression (8), the bending moment M_z can be expressed as

$$M_z(y) = EJ_z \frac{d^2 u}{dy^2}.$$
(9)

On the other hand, M_z is a moment of forces with respect to point y due to the action of force F_z $(M_{F_z} = F_z(l-y))$ and the beam own weight $(M_{mg} = -\frac{mg}{l}\int_y^l pdp = -\frac{mg}{2l}(l^2 - y^2))$. Thus,

$$\frac{d^2 u}{dy^2} = \frac{F_z}{EJ_z} (l - y) - \frac{mg}{2lEJ_z} (l^2 - y^2).$$
(10)

Integration of (10) having for boundary conditions $u\Big|_{y=0} = 0$ and $\frac{du}{dy}\Big|_{y=0} = 0$, gives:

$$u(y) = \frac{F_z}{6EJ_z} (3l - y)y^2 - \frac{mg}{24lEJ_z} (6l^2 - y^2)y^2.$$
(11)

The beam end deflection Δz is (Fig. 2):

$$\Delta z = u \Big|_{y=l} = \frac{F_z l^3}{3EJ_z} - \frac{5mgl^3}{24EJ_z}.$$
 (12)

The second summand is the deflection under own weight. For a typical cantilever, it is of the fraction of the angstrom and can be neglected because in AFM experiments the first term is hundreds of time more.

Relation (12) is nothing but expression (6) in which we should suppose:

$$c_{zz} = \frac{l^3}{3EJ_z} = c.$$
 (13)

The beam deflection angle calculated without the second term in (12) is as follows:

$$\alpha \approx \operatorname{tg} \alpha = \frac{du}{dy}\Big|_{y=l} = \frac{F_z l^2}{2EJ_z} = \frac{3}{2} \frac{\Delta z}{l} = \frac{3}{2} cF_z \,. \tag{14}$$

The coefficient of inverse stiffness c_{zz} is the largest among the tensor C components. In (13) this parameter is specially denoted as "c" without indexes. In particular, magnitude of 1/c characterizes the cantilever stiffness and is one of its major parameters. Below, for the purpose of obviousness, we will take c outside as a common multiplier of all the matrix (2) (section 2.1.1) components. For a cantilever with rectangular cross-section, (13) can be rewritten as

$$c = \frac{4l^3}{Ewt^3}.$$
(15)

From formula (14) and diagram for the beam vertical bending of z-type (Fig. 2) it is easy to derive the tip deflection Δy induced by the force F_z application:

$$\Delta y = \alpha \cdot l_{tip} = \frac{3}{2} \frac{l_{tip}}{l} \Delta z \,. \tag{16}$$

From (16) and (4)-(6) it is clear that

$$c_{yz} = \frac{3}{2} \frac{l_{tip}}{l} c \quad . \tag{17}$$

Taking into consideration that $\Delta x = 0$, we get

$$c_{xz} = 0. (18)$$

Finally, we calculate the components of the matrix (3) third column. From expressions (13)-(15) it follows that

$$b_{\alpha z} = \frac{3}{2l}c.$$
⁽¹⁹⁾

Because under the influence of the force F_z the top cantilever surface does not bend in the Oxz direction, then

$$b_{\beta z} = 0. \tag{20}$$

- 1. The *z*-type deflection is a result of the vertical bending force action.
- 2. To find the components of the inverse stiffness tensor corresponding to the *z*-type deflection, one should solve the problem of the beam static deflection which is reduced to the ordinary differential equation of the second order.
- 3. The vertical force results in the tip deflection in vertical and longitudinal directions and in the deflection angle $\alpha = \frac{l^2}{2EJ_z}F_z = \frac{3}{2l}cF_z$ appearance.
- 4. Besides the supporting force from the sample, the cantilever is influenced in vertical direction by its own gravity. Under this load the cantilever free end is deflected but such a deformation is small compared to minimal detected displacement.

2.1.3 Deflections under the longitudinal force (F_{y})

In this section we determine the magnitude and direction of the deformation produced by the axial force F_{y} . Solution to this problem will give the middle column (2) of tensor C.

$$\Delta x = c_{xy} F_y, \qquad (21)$$

$$\Delta y = c_{yy} F_y, \qquad (22)$$

$$\Delta z = c_{zy} F_y \,. \tag{23}$$

The force F_y acting in the cantilever axis direction produces moment $M = F_y l_{tip}$ that results in deformation called here the vertical bending of y-type (Fig. 4).



Fig. 4. Vertical deflection of the *y*-type

In spite of the formal resemblance to vertical bending of z-type (see section 2.1.2), the deformation profile in this case is quite different. The equation describing the y-type bending reads

$$\frac{d^2u}{dy^2} = \frac{F_y l_{tip}}{EJ_z}.$$
(24)

Boundary conditions remain the same: $u\Big|_{y=0} = 0$ and $\frac{du}{dy}\Big|_{y=0} = 0$. For the solution we find:

$$u(y) = \frac{F_{y} l_{tip}}{2EJ_{z}} y^{2}.$$
 (25)

Thus, the tip vertical deflection due to this type of deformation is as follows:

$$\Delta z = u(l) = \frac{F_y l_{ip} l^2}{2EJ_z} = \frac{3}{2} \frac{l_{ip}}{l} cF_y.$$
(26)

Comparing (26) and (23) and taking into account the expression for the common multiplier c (13), we get:

$$c_{zy} = \frac{l_{tip}l^2}{2EJ_z} = \frac{3l_{tip}}{2l}c.$$
 (27)

The angle of the beam end deflection α is given by the following formula:

$$\alpha = \frac{du}{dy}\Big|_{y=l} = \frac{F_y l_{iip} l}{EJ_z} = 2\frac{\Delta z}{l} = \frac{3l_{iip}}{l^2} cF_y.$$
(28)

From formula (28) and diagram for the beam vertical bending of *y*-type (Fig. 4) it is easy to derive the tip deflection Δy induced by the force F_y application:

$$\Delta y = \alpha \, l_{iip} = \frac{2 l_{iip}}{l} \Delta z \,. \tag{29}$$

From (22), (27) and (29) it is easy to obtain:

$$c_{yy} = \frac{2l_{tip}}{l}c_{zy} = \frac{3l_{tip}^{2}}{l^{2}}c.$$
 (30)

Taking into account that $\Delta x = 0$, we get:

$$c_{xy} = 0. ag{31}$$

Finally, we calculate the components of the matrix (3) third column. From expressions (25)-(27) it follows that

$$b_{ay} = \frac{3l_{tip}}{l^2}c.$$
(32)

Because under the influence of the force F_y the top cantilever surface does not bend in the Oxz direction, then

$$b_{\beta \gamma} = 0. \tag{33}$$

- 1. The *y*-type deflection is a result of the axial bending force action.
- 2. To find the components of the inverse stiffness tensor corresponding to the *y*-type deflection, one should solve the problem of the beam static deflection which is reduced to the ordinary differential equation of the second order.
- 3. The axial force results in the tip deflection not only in the longitudinal but also in vertical direction $\Delta z = \frac{3}{2} \frac{l_{tip}}{l} cF_y$ and in the deflection angle $\alpha = \frac{l_{tip}l}{EJ_z} F_y = \frac{3l_{tip}}{l^2} cF_y$ appearance.

2.1.4 Deflections under the transverse force (F_x)

In this section we determine the magnitude and direction of the deformation produced by the transverse force F_y . Solution to this problem will give the first column of tensor C (2) components.

$$\Delta x = c_{\rm yy} F_{\rm y}, \tag{34}$$

$$\Delta y = c_{yx} F_x, \qquad (35)$$

$$\Delta z = c_{xx} F_{x} \,. \tag{36}$$

As a result of the transverse force action, the complicated deformation is induced which is a superposition of simple bending and twisting (Fig. 5a and 5b).



Fig. 5a. Simple bending



It is easy to obtain the inverse stiffness of simple bending (Fig.5a). This deformation is analogous to the vertical bending of z-type (Fig. 2 in section 2.1.2) with the only difference that in final expression for the inverse stiffness (15) we must interchange the beam width with its thickness $(w \leftrightarrow t)$:

$$c_{bend} = \frac{4l^3}{Ew^3 t} = \frac{t^2}{w^2} c .$$
(37)

The solution to the problem of the rectangular beam torsion is much more complicated. Therefore, we give the formula relating the torsion angle β and applied to the beam end force moment *M* [4] without derivation:

$$\beta = \frac{3lM}{Gwt^3},\tag{38}$$

where G – shear modulus.

If the lateral force F_x acts on the tip having length l_{tip} then torque is given by $M = F_x l_{tip}$. The tip lateral deflection is, in turn, related with the torsion angle as $\Delta x_{tors} = \beta l_{tip}$. Hence, the inverse stiffness coefficient reads:

$$c_{tors} = \frac{\Delta x_{tors}}{F_x} = \frac{3l_{tip}^2 l}{Gwt^3}.$$
(39)

Knowing that $G = \frac{E}{2(1+v)}$, the Poisson's ratio is $v \approx 1/3$ (for the majority of materials) and

taking into account the expression for c (15), the coefficient is calculated as:

$$c_{tors} \approx \frac{8l_{tip}^{2}l}{Ewt^{3}} = \frac{2l_{tip}^{2}}{l^{2}}c.$$
 (40)

To find the resulting tip deflection at superposition of simple bending and torsion it is just enough to sum the corresponding deflections (assuming that deformations are small):

$$\Delta x = \Delta x_{bend} + \Delta x_{tors} = c_{bend} F_x + c_{tors} F_x = c_{xx} F_x \,. \tag{41}$$

Thus, the resulting inverse stiffness is a sum of the simple bending and torsion inverse stiffness, too:

$$c_{xx} = \left(\frac{2l_{tip}^{2}}{l^{2}} + \frac{t^{2}}{w^{2}}\right) \cdot c.$$
(42)

Note that for the most of cantilevers the simple bending inverse stiffness c_{bend} (37) exceeds much the torsion inverse stiffness c_{tors} (40) so normally the simple bending can be neglected. For the standard AFM cantilever CSC12 having the following parameters: l = 90 MKM, $l_{tip} = 10 \text{ MKM}$, w = 35 MKM, t = 1 MKM, stiffness 1/c = 0.52 H/M, the lateral stiffness constants are:

$$c_{tors} \approx \frac{1}{40} c \approx 0.05 \frac{M}{H}, \ c_{bend} \approx \frac{1}{1220} c \approx 0.0016 \frac{M}{H}.$$
 (43)

Notice that besides the Δx deflection, both the simple bending and torsion induce the deformations Δy and Δz , respectively. However, the magnitude of these displacements is of the next order of smallness as compared with Δx and their relation with applied force is nonlinear (quadratic), i.e. "non-Hookean". We can prove this, e.g. for torsion.



Referring to Fig. 6, we can write:

$$\Delta z = l_{tip} \left(1 - \cos \beta \right) \approx l_{tip} \frac{\beta^2}{2}, \qquad (44)$$

while:

$$\Delta x = l_{tip} \cdot \beta \,. \tag{45}$$

Since $\beta \ll 1$, then $\Delta z \ll \Delta x$. Similarly, at the simple bending $\Delta y \ll \Delta x$. Hence, we can suppose:

$$c_{yx} = c_{zx} = 0. (46)$$

Finally, we calculate the components of the first matrix (2) column. The normal to the top surface of the cantilever, subjected to the transverse force F_x , deflects in the Oxz plane, so from (44)-(46) we can derive:

$$b_{\beta x} = \frac{2l_{tip}}{l^2} c \,. \tag{47}$$

Accordingly, there is no deflection in the Oyz direction, so:

$$b_{ax} = 0. (48)$$

Note that nonzero angle β arises only from the torsional deformation. At the simple bending the cantilever surface remains horizontal so this bending can not be detected and its magnitude can only be calculated. However, to determine the transverse force experimentally, it is enough to detect the torsional deformation.

- 1. The transverse force results in a complicated deformation which is a superpositon of the simple bending and torsion of the cantilever beam. The simple bending is analogous to the *z*-type deflection. Solution to the more difficult problem of the rectangular beam torsion is given in literature [4].
- 2. Only transverse deflection of the cantilever tip (in the first order of smallness according to the Hooke's law) occurs as a result of the transverse force action.
- 3. The optical detection system registers only torsional deformation $\beta = \frac{2l_{tip}}{l^2} cF_x$. The simple bending can not be measured directly.

2.1.5 Cantilever inverse stiffness tensor

Let us write the obtained components of inverse stiffness tensor C (2) into the representative matrix for mathematical convenience:

$$\mathbf{C} = \begin{pmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{pmatrix}.$$

The (x,x) coefficient of inverse stiffness - c_{zz} is the largest of other tensor C components. In formula (13) this parameter is specially denoted as c without indexes. It is namely the quantity 1/c that characterizes a cantilever stiffness which is one of its major parameters. Below, for the sake of clearness, we will take c outside as a common multiplier of all the matrix elements [1]:

$$\mathbf{C} = c \cdot \begin{pmatrix} \frac{2l_{iip}^{2}}{l^{2}} + \frac{t^{2}}{w^{2}} & 0 & 0\\ 0 & \frac{3l_{iip}^{2}}{l^{2}} & \frac{3l_{iip}}{2l}\\ 0 & \frac{3l_{iip}}{2l} & 1 \end{pmatrix}.$$
 (49)

Tensor C is symmetric. That is true. The left side of expression (1) in section 2.1.1, Δ , is a polar vector, therefore, the right side must have the same transformational properties. The force F is a polar vector; therefore, the tensor must be symmetric in order to properly transform the expression (1) at co-ordinates reflections.

The presence of non-diagonal elements leads to the difference in directions of the applied force and of the tip deflection vector and is an evidence of limited applicability of the elastic cantilever simplified model based on three perpendicular springs. To apply this model, one should determine not only stiffness but true directions of three springs that do not coincide with coordinate axes. This problem is reduced to the tensor (49) diagonalization in order to obtain its eigenvalues as well as to determine the directions of transformed co-ordinates along which the model springs should be oriented.

It is seen that the cantilever elastic properties are completely defined by five parameters. We can find all tensorial components knowing geometrical characteristics of the cantilever and its stiffness constant.

To facilitate computation at experiments, the obtained components are introduced into the matrix in formula (3) of section 2.1.1:

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = c \cdot \begin{pmatrix} 0 & \frac{3l_{tip}}{l^2} & \frac{3}{2l} \\ \frac{2l_{tip}}{l^2} & 0 & 0 \end{pmatrix} \begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}.$$
 (50)

- 1. The tensor component c_{zz} corresponding to the vertical displacement at z-type deflection is the largest. Its inverse value is the beam stiffness constant that characterizes a cantilever.
- 2. Tensorial nature of a cantilever elastic properties leads to the limited applicability of simplified models based on springs.
- 3. To properly model a cantilever elastic properties by three springs, one should determine their parameters correctly by diagonalization of the inverse stiffness tensor.

2.1.6 Effective mass and eigenfrequency of the cantilever

In AFM, there exist techniques that are based not only on static beam deflection detection but also on cantilever vibration. To use them one should know the cantilever resonant frequency.

Let us calculate the resonant frequency of isotropic cantilever with mass m in the form of parallepiped having length l, thickness h ($h \ll l$) and width w ($w \ll l$) to the free end of which the vertical point force F is applied (see Fig. 7).



Fig. 7. Rectangular cantilever with a tip

Determine kinetic $E_{\kappa un}$ and potential E_{nom} energy of the cantilever. Consider the beam element having length dy at distance y from the fixed end. Kinetic energy of such an element is given by:

$$dE_{_{\kappa u \mu}} = \frac{\left(\dot{u}\left(\tau, y\right)\right)^2}{2} \frac{m dy}{l},\tag{51}$$

where $u(\tau, y)$ — displacements of the beam axial points at distance y from the fixed end at time τ . Using formulas (11), (12) of section 2.1.2, $u(\tau, y)$ can be obtained as a function of the beam free end deflection $u(\tau, l)$:

$$u(\tau, y) = \frac{u(\tau, l)}{2} \left(3 \left(\frac{y}{l} \right)^2 - \left(\frac{y}{l} \right)^3 \right).$$
(52)

Substituting the expression for $u(\tau, y)$ into (51) and integrating over the beam length, we get:

$$E_{\kappa u \mu} = \int_{0}^{L} \frac{\left(\dot{u}(\tau, y)\right)^{2}}{2} \frac{m dy}{l} = \frac{33}{140} \frac{m}{2} \left(\dot{u}(\tau, l)\right)^{2}.$$
(53)

Potential energy calculation is easier. Because the point force F acts only on the free end, E_{nom} is evidently equal to the work done to move the beam end the distance $u(\tau, l)$:

$$E_{nom} = \int_{0}^{u(\tau,l)} F du = \int_{0}^{u(\tau,l)} \frac{1}{c} u du = \frac{u^2(\tau,l)}{2c},$$
(54)

where 1/c — coefficient of normal stiffness defined by formula (13).

If system vibrations are considered to occur without total energy W dissipation, i.e. $W = E_{\kappa un} + E_{nom} = const$, then, differentiating W with respect to time, we get equation of the cantilever free end move:

$$\frac{33mu(\tau,l)}{140} + \frac{1}{c}u(\tau,l) = 0.$$
(55)

Therefore, the cantilever effective mass is:

$$m_{_{}^{}_{\phi\phi\phi}} = \frac{33}{140} m \,. \tag{56}$$

Thus, calculating $m_{_{3\phi\phi}}$ and knowing the coefficient of stiffness 1/c defined by formula (15) in section 2.1.2 the eigenfrequency of the cantilever oscillation can be expressed as a function of its parameters in the following way:

$$\omega_0 = \sqrt{\frac{1}{cm_{s\phi\phi}}} = \frac{1.029t}{l^2} \sqrt{\frac{E}{\rho}} , \qquad (57)$$

where ρ — cantilever density, E — Young's modulus. As can be seen from (6), ω_0 is inversely as the square of the beam length. This fact should be taken into consideration when choosing a cantilever. The cantilever eigenfrequency must be as high as possible, otherwise its natural oscillations will be readily excited due to the probe trace-retrace move during scanning or due to external vibrations influence.

- 1. To employ AFM techniques based on the probe vibration, one should know the cantilever eigenfrequency and effective mass.
- 2. The effective mass is given by: $m_{_{2}\phi\phi} = \frac{33}{140}m$.
- 3. The eigenfrequency is: $\omega_0 = \frac{1.029t}{l^2} \sqrt{\frac{E}{\rho}}$.

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