EXACT ANALYTICAL SOLUTION FOR ELECTROSTATIC FIELD PRODUCED BY BIASED ATOMIC FORCE MICROSCOPE TIP DWELLING ABOVE DIELECTRIC-CONDUCTOR BI-LAYER

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Abstract. An exact analytical solution based on the method of images has been obtained for the description of the electrostatic field in the system consisting of atomic force microscope (AFM) tip, dielectric and conductor. The solution provides a step towards quantitative modelling of the AFM-assisted electrostatic nanolithography in polymers.

1. Introduction

Atomic Force Microscopy is an important tool for nanoscale modifications in metals, semiconductors, and soft condensed matter. Polymers suggest clear advantage with respect to the other materials in such fields as data storage and sacrificial patterning. Recently, an electrostatic nanolithography based on AFM [1,2] suggested a way of patterning nanostructures in thin (10-50 nm) dielectric films coated onto metal substrate. Although the physical description of the process based on electrostatic attraction of softened polymer toward the tip in strong non-uniform electric field has apparently been understood, the mathematical model has not been developed until this time.

The goal of this Letter is to derive the exact analytical solution for the spatial distribution of the electric field and potential in the system consisting of a biased AFM tip, dielectric polymer film, and a conductor using the method of images. This solution is required for phenomenological description of the tip-polymer interaction and electrostatic pressure formed inside the softened dielectric material. The model we introduce differs from that considered in [3] due to the presence of a conductive substrate.

2. Model description. Field equations and boundary conditions

A conceptual presentation of the system comprising conductive AFM tip and bi-layer consisting of the polymer film and conductive substrate is shown in Figure 1. An electrically biased AFM tip is presented as an equipotential spherical surface, modelled by a charge Q in its center. An opposite charge of planar density σ is distributed over the surface of the dielectric film.

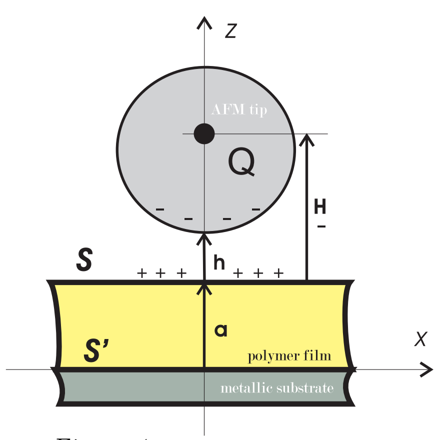

Figure 1

The electric field $\mathbf{E} = \mathbf{E}(\mathbf{r})$, produced by Q and σ, should satisfy the following electrostatic equations [4]:

$$\operatorname{rot} \mathbf{E} = 0, \qquad \operatorname{div} \mathbf{E} = 0. \tag{2.1}$$

The electric field inside the bulk conductor equals zero: $\mathbf{E}(\mathbf{r}) = 0$ for $z < 0$. The field is perpendicular to the conductor - dielectric interface S':

$$\mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S'} = 0. \tag{2.2}$$

The tangential component of $\mathbf{E}$ is continuous at the interface S, while normal components of the electric field $\mathbf{E}$ and the electric displacement vector $\mathbf{D}$ undergo a discontinuity related to σ:

$$\mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S-0} = \mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S+0}, \qquad \mathbf{D}_{\perp}\Big|_{\mathbf{r}\in S-0} + \sigma = \mathbf{D}_{\perp}\Big|_{\mathbf{r}\in S+0}. \tag{2.3}$$

For the linear dielectric media, $\mathbf{D}$ is linearly proportional to $\mathbf{E}$:

$$\mathbf{D} = \begin{cases} \epsilon_0\, \varepsilon_{\text{air}}\, \mathbf{E} & \text{for } \ z > a \ \text{ above } S, \\ \epsilon_0\, \varepsilon_{\text{pol}}\, \mathbf{E} & \text{for } \ 0 < z < a \ \text{ below } S. \end{cases} \tag{2.4}$$

Here ε_{air} and ε_{pol} are the dielectric constants of air and polymer film respectively. The second boundary condition (2.3) can be rewritten as

$$\varepsilon_{\text{pol}}\, \mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S-0} + \frac{\sigma}{\epsilon_0} = \varepsilon_{\text{air}}\, \mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S+0}. \tag{2.5}$$

The combination of (2.5) and the first part of (2.3),

$$\mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S-0} = \mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S+0}, \qquad \varepsilon_{\text{pol}}\, \mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S-0} + \frac{\sigma}{\epsilon_0} = \varepsilon_{\text{air}}\, \mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S+0}, \tag{2.6}$$

along with (2.2), provide the boundary conditions for the differential equations (2.1).

3. Basic (auxiliary) electrostatic field in air

In the general case, the charge density distribution σ on the polymer surface depends on the tip's motion with respect to the polymer surface. The axially symmetric σ is given by

$$\sigma(r) = \frac{-Q'\, k\, H}{2\,\pi\,(k^2\, H^2 + r^2)^{3/2}}, \quad \text{where} \quad r = \sqrt{x^2 + y^2}. \tag{3.1}$$

The total charge, distributed on the polymer surface, equals $-Q'$:

$$2\pi \int\limits_0^{\infty} \sigma(r)\, r\, dr = -Q'.$$

The degree of spatial concentration of the surface charge density can be varied adjusting the parameter $k > 0$ in (3.1).

It is convenient to use the following auxiliary construction in the derivation of the electrostatic field distribution for the system of our interest. If we consider the system of the point charge Q and charge density $\sigma(r)$ at the absence of the dielectric and conductor, the electrostatic field is given by

$$\mathbf{E}_{\text{bas}}(\mathbf{r}) = \begin{cases} \dfrac{Q}{4\,\pi\,\epsilon_0\,\varepsilon_{\text{air}}}\, \dfrac{\mathbf{r} - \mathbf{r}_Q}{|\mathbf{r} - \mathbf{r}_Q|^3} - \dfrac{Q'}{4\,\pi\,\epsilon_0\,\varepsilon_{\text{air}}}\, \dfrac{\mathbf{r} - \mathbf{r}'_Q}{|\mathbf{r} - \mathbf{r}'_Q|^3} & \text{below } \ S, \\[2ex] \dfrac{Q}{4\,\pi\,\epsilon_0\,\varepsilon_{\text{air}}}\, \dfrac{\mathbf{r} - \mathbf{r}_Q}{|\mathbf{r} - \mathbf{r}_Q|^3} - \dfrac{Q'}{4\,\pi\,\epsilon_0\,\varepsilon_{\text{air}}}\, \dfrac{\mathbf{r} - \mathbf{r}''_Q}{|\mathbf{r} - \mathbf{r}''_Q|^3} & \text{above } \ S. \end{cases} \tag{3.2}$$

Here $\mathbf{r}_Q = \mathbf{a} + \mathbf{H}$, $\mathbf{r}_{Q'} = \mathbf{a} + k\,\mathbf{H}$ and $\mathbf{r}_{Q''} = \mathbf{a} - k\,\mathbf{H}$ are radii-vectors of the actual charge Q, and the virtual (image) charges $-Q'$, placed below the interface S. Below, we modify the basic electrostatic field (3.2) to describe the case when the dielectric - conductor bi-layer is placed below S.

4. Solution of the original electrostatic problem

The problem is to construct the actual electric field distribution $\mathbf{E}(\mathbf{r})$ for the case when an external field $\mathbf{E}_{\text{bas}}(\mathbf{r})$ applies to the dielectric - conductor bi-layer. To solve this problem we use the method of images [4]. A discrete set of vectors is introduced in the following form:

$$\mathbf{a}_n = 2\,n\,\mathbf{a}, \qquad n = 0, 1, 2, \dots, \infty. \tag{4.1}$$

Reflection operator acts

$$\mathbf{r} = \left\| \begin{matrix} x \\ y \\ z \end{matrix} \right\| \longrightarrow \overline{\mathbf{r}} = \left\| \begin{matrix} x \\ y \\ -z \end{matrix} \right\|. \tag{4.2}$$

The reflection operation is denoted by the bar above the vector. We seek solution for the electric field inside the polymer film in the form

$$\mathbf{E}(\mathbf{r}) = \sum_{n=0}^{\infty} \alpha_n\, \mathbf{E}_{\text{bas}}(\mathbf{r} - \mathbf{a}_n) - \sum_{n=0}^{\infty} \alpha_n\, \overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_n). \tag{4.3}$$

The form of the sum (4.3) satisfies the boundary condition (2.2) for the conductor - dielectric interface S'. For a point at S', $\overline{\mathbf{r}} = \mathbf{r}$, and $\mathbf{E}_{\text{bas}}(\mathbf{r} - \mathbf{a}_n) = \mathbf{E}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_n)$. Hence,

$$\mathbf{E}^{\parallel}_{\text{bas}}(\mathbf{r} - \mathbf{a}_n)\Big|_{\mathbf{r}\in S'} = \overline{\mathbf{E}}^{\parallel}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_n)\Big|_{\mathbf{r}\in S'}, \tag{4.4}$$

and continuity of the tangential component of the electric field is satisfied.

Now, the components of the electric field $\mathbf{E}_{\parallel}$ and $\mathbf{E}_{\perp}$ at the interface S of the polymer film can be found. For the point $\mathbf{r} \in S$, $\overline{\mathbf{r}} = \mathbf{r} - 2\,\mathbf{a}$; thus, $\overline{\mathbf{r}} - \mathbf{a}_n = \mathbf{r} - \mathbf{a}_{n+1}$ and the following relationship holds:

$$\mathbf{E}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_n)\Big|_{\mathbf{r}\in S} = \mathbf{E}_{\text{bas}}(\mathbf{r} - \mathbf{a}_{n+1})\Big|_{\mathbf{r}\in S}. \tag{4.5}$$

The following notations are introduced for convenience:

$$G^{\parallel}_n = \mathbf{E}^{\parallel}_{\text{bas}}(\mathbf{r} - \mathbf{a}_n)\Big|_{\mathbf{r}\in S}, \qquad G^{\perp}_n = \mathbf{E}^{\perp}_{\text{bas}}(\mathbf{r} - \mathbf{a}_n)\Big|_{\mathbf{r}\in S}. \tag{4.6}$$

Using (4.3), (4.5), (4.6) and (4.2), the following two expressions for normal and tangential field components can be written:

$$\mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S-0} = \alpha_0\, G^{\parallel}_0 + \sum_{n=0}^{\infty} (\alpha_{n+1} - \alpha_n)\, G^{\parallel}_{n+1}, \tag{4.7}$$

$$\mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S-0} = \alpha_0\, G^{\perp}_0 + \sum_{n=0}^{\infty} (\alpha_{n+1} + \alpha_n)\, G^{\perp}_{n+1}. \tag{4.8}$$

The electric field above the boundary S is presented as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\text{bas}}(\mathbf{r} - \mathbf{a}_0) + \beta_{-1}\, \overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_{-1}) + \sum_{n=0}^{\infty} \beta_n\, \overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}} - \mathbf{a}_n). \tag{4.9}$$

Combining (4.5), (4.6) and (4.2) with (4.9) we find

$$\mathbf{E}_{\parallel}\Big|_{\mathbf{r}\in S+0}=(1+\beta_{-1})\,G_0^{\parallel}+\sum_{n=0}^{\infty}\beta_n\,G_{n+1}^{\parallel},\tag{4.10}$$

$$\mathbf{E}_{\perp}\Big|_{\mathbf{r}\in S+0}=G_0^{\perp}-\beta_{-1}\,G_0^{\perp}-\sum_{n=0}^{\infty}\beta_n\,G_{n+1}^{\perp},\tag{4.11}$$

Considering (4.7), (4.8) and (4.10), (4.11) simultaneously, together with the boundary conditions (2.6), the relationships for series coefficients can be found:

$$\begin{cases}1+\beta_{-1}=\alpha_0,\\ \varepsilon_{\text{air}}\,(1-\beta_{-1})=\varepsilon_{\text{pol}}\,\alpha_0.\end{cases}\tag{4.12}$$

and

$$\begin{cases}\beta_n=\alpha_{n+1}-\alpha_n,\\ -\varepsilon_{\text{air}}\,\beta_n=\varepsilon_{\text{pol}}\,(\alpha_{n+1}+\alpha_n),\end{cases}\qquad n=0,1,\ldots,\infty.\tag{4.13}$$

Note, that the basic field (3.2) undergoes discontinuiety at the interface S. Two different values of $G_0^{\perp}$ are obtained from (4.8) and (4.11):

$$G_0^{\perp}(+)=\mathbf{E}_{\text{bas}}^{\perp}(\mathbf{r}-\mathbf{a}_0)\Big|_{\mathbf{r}\in S+0},\qquad\qquad G_0^{\perp}(-)=\mathbf{E}_{\text{bas}}^{\perp}(\mathbf{r}-\mathbf{a}_0)\Big|_{\mathbf{r}\in S-0}.$$

The difference of these two values is related to the surface charge density σ:

$$G_0^{\perp}(+)-G_0^{\perp}(-)=\frac{\sigma}{\epsilon_0\,\varepsilon_{\text{air}}}.\tag{4.14}$$

Solving (4.12) and (4.13) for the series coefficients α_n and β_n, we can find the recurrent relationships

$$\alpha_{n+1}=-\frac{\varepsilon_{\text{pol}}-\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}\,\alpha_n,\qquad\qquad\beta_n=-\frac{2\,\varepsilon_{\text{pol}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}\,\alpha_n,\tag{4.15}$$

and

$$\alpha_0=\frac{2\,\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}},\qquad\qquad\beta_{-1}=-\frac{\varepsilon_{\text{pol}}-\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}.\tag{4.16}$$

From (4.15) and (4.16), we finally obtain the explicit expressions for the series coefficients:

$$\begin{aligned}\alpha_n&=\left(-\frac{\varepsilon_{\text{pol}}-\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}\right)^{n}\,\frac{2\,\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}},\\ \beta_n&=-\left(-\frac{\varepsilon_{\text{pol}}-\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}\right)^{n}\,\frac{4\,\varepsilon_{\text{pol}}\,\varepsilon_{\text{air}}}{(\varepsilon_{\text{pol}}+\varepsilon_{\text{air}})^2}\end{aligned}\tag{4.17}$$

Introducing

$$\eta=\frac{\varepsilon_{\text{pol}}-\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}},\tag{4.18}$$

and noting that

$$\frac{\varepsilon_{\text{air}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}=\frac{1-\eta}{2},\qquad\qquad\frac{\varepsilon_{\text{pol}}}{\varepsilon_{\text{pol}}+\varepsilon_{\text{air}}}=\frac{1+\eta}{2},\tag{4.19}$$

we have

$$\alpha_0 = 1-\eta, \qquad \beta_{-1} = -\eta, \tag{4.20}$$

$$\alpha_n = (-\eta)^n\,(1-\eta), \qquad \beta_n = -(-\eta)^n\,(1-\eta^2). \tag{4.21}$$

Finally, the electrostatic field inside the polymer, and above the polymer film is given by

$$\mathbf{E}(\mathbf{r}) = (1-\eta)\sum_{n=0}^{\infty}(-\eta)^n\left(\mathbf{E}_{\text{bas}}(\mathbf{r}-\mathbf{a}_n) - \overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}}-\mathbf{a}_n)\right), \tag{4.22}$$

$$\begin{aligned}\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\text{bas}}(\mathbf{r}-\mathbf{a}_0) - \eta\,\overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}}-\mathbf{a}_{-1}) - \\ -(1-\eta^2)\sum_{n=0}^{\infty}(-\eta)^n\,\overline{\mathbf{E}}_{\text{bas}}(\overline{\mathbf{r}}-\mathbf{a}_n).\end{aligned} \tag{4.23}$$

5. Induced charges

The electric field polarizes polymer film with the degree of polarization described through the induced density of the dipole moment $\mathbf{P}$. Vector $\mathbf{P}$ is given by

$$\begin{aligned}\mathbf{P}_{\text{air}} &= \epsilon_0\,(\varepsilon_{\text{air}}-1)\,\mathbf{E}_{\text{air}},\\ \mathbf{P}_{\text{pol}} &= \epsilon_0\,(\varepsilon_{\text{pol}}-1)\,\mathbf{E}_{\text{pol}}.\end{aligned} \tag{5.1}$$

The bulk and the surface charge distributions appear as a result of polarization induced by the electric field:

$$\rho = -\operatorname{div}\mathbf{P}, \qquad \sigma = \mathbf{P}\cdot\mathbf{n}, \tag{5.2}$$

for the volume and surface charge densities. Here $\mathbf{n}$ is the unit vector normal to the interface S. The constancy of the dielectric constants ε_{pol} and ε_{air} yields $\operatorname{div}\mathbf{D} = 0$ and $\operatorname{div}\mathbf{E} = 0$. This implies no volume electric charges inside the polymer film. Using Gauss' theorem, the electric field due to the surface charge on the interface S is presented as

$$\mathbf{E}_\sigma\Big|_{\mathbf{r}\in S+0} - \mathbf{E}_\sigma\Big|_{\mathbf{r}\in S-0} = \frac{\sigma}{\epsilon_0}\,\mathbf{n}. \tag{5.3}$$

This field must be subtracted from the expression for the net electrostatic field, given by (4.22) and (4.23), in order to exclude self-action when calculating tension forces and pressure associated with the field. The resulting function $\mathbf{E}(\mathbf{r}) - \mathbf{E}_\sigma(\mathbf{r})$ is continuous on S, and its value on S is

$$(\mathbf{E}-\mathbf{E}_\sigma)\Big|_{\mathbf{r}\in S} = \frac{\mathbf{E}(\mathbf{r})}{2}\Big|_{\mathbf{r}\in S+0} + \frac{\mathbf{E}(\mathbf{r})}{2}\Big|_{\mathbf{r}\in S-0} = \mathbf{E}_{\text{av}}. \tag{5.4}$$

The traction acting on the upper surface of the polymer film, related to the stress induced by the electrostatic field, is

$$\mathbf{T} = \sigma\mathbf{E}_{\text{av}}. \tag{5.5}$$

The surface density of polarization charges is expressed through the electric field inside the polymer film, (4.22), according to (5.2) and (5.3), as

$$\sigma_{\text{pol}} = \epsilon_0\,(\varepsilon_{\text{pol}}-1)\,\mathbf{E}^{\perp}_{\text{pol}}. \tag{5.6}$$

Summary

The exact analytical solution for a spatial distribution of the electrostatic field in the system consisting of the electrically biased AFM tip and the dielectric - conductor bi-layer has been derived. The solution has been developed in the series form using the method of images. The expressions have been obtained for the charge density and traction of the electrostatic stress at the polymer surface. Represented results provide a step towards the quantitative understanding of the AFM-assisted electrostatic nanolithography in polymers.

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