The resolution function and effective response of piezoelectric thin films in Piezoresponse Force Microscopy

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Abstract. The elastic Green function and resolution function in Piezoresponse Force Microscopy (PFM) of thin piezoelectric film capped on the rigid substrate are derived. The extrinsic size effect on the resolution function is demonstrated.

Keywords: Piezoresponse Force Microscopy, thin piezoelectric films, resolution function.

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1. Introduction

Verification of existing theoretical models, design of functional nanomaterials with predetermined properties, and application in various devices necessitate experimental and theoretical studies of piezoelectric coupling and ferroelectric properties in surface layers. These considerations of the local polarization switching behavior in thin films are possible in the context of Piezoresponse Force Microscopy (PFM) [1, 2].

Conventional framework for the PFM data analysis was based on the 1D models suggested originally by Ganpule, thus ignoring the 3D geometry of the PFM problem. Only recently, the decoupled theory [3, 4] was applied to derive analytical expressions for PFM response on semi-infinite materials of low symmetry, derive analytical expressions for resolution function and domain wall profiles, and interpret PFM spectroscopy data [5].

Further, the local piezoresponse dependence on film thickness was predicted in [6] for thin films capped on the nonpiezoelectric bulk with the same elastic and close dielectric properties. In the paper, the complementary case of thin piezoelectric films capped on rigid substrates is considered within the framework of decoupled approximation. For ferroelectric perovskite films like BaTiO₃ or Pb(Ti, Zr)O₃ rigid dielectric substrates are MgO oxide, sapphire Al₂O₃ or carbon with effective dielectric constant \( \kappa_b \approx 10^5 \). Silicon (\( \kappa_b \approx 3–12 \)) and SiO₂ (\( \kappa_b \approx 5 \)) have smaller elastic stiffness than typical perovskites.

2. Elastic Green function of thin film on rigid substrate

Let us derive the elastic Green function for the layer on the rigid substrate. General equation for the field of elastic displacement vector is [7]:

\[
\Delta_x u + \frac{1}{1-2\nu} \text{grad}_x (\text{div}_x u) = -\frac{2(1+\nu)}{Y} F \cdot \delta(x - \xi).
\]

(1a)

Here the vector \( x \) denotes the given location and \( \xi \) is the point at which the point force, \( F \), is applied. The material is isotropic and \( \nu \) is the Poisson coefficient, \( Y \) is the Young modulus. Introducing the shear modulus \( \mu = Y/(2(1+\nu)) \), Eq. (1a) can be rewritten as:

\[
\frac{\partial^2 u_i}{\partial x_k \partial x_k} + \frac{1}{1-2\nu} \frac{\partial^2 u_m}{\partial x_i \partial x_m} = -\frac{F_i}{\mu} \delta(x - \xi).
\]

(1b)

Introducing transversal Fourier transformation

\[
\tilde{u}_i(k_1, k_2, x_3) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \exp(ik_1 x_1 + ik_2 x_2) u_i(x),
\]

(2a)

\[
u_i(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2 \exp(-ik_1 x_1 - ik_2 x_2) \tilde{u}_i(k_1, k_2, x_3),
\]

(2b)
and using integral representation of the delta function
\[
\begin{align*}
\delta(x_1 - \xi_1)\delta(x_2 - \xi_2) &= \\
= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dk_1dk_2 \exp(-ik_1(x_1 - \xi_1) - ik_2(x_2 - \xi_2)).
\end{align*}
\]

Eq. (1b) yields:
\[
\begin{align*}
-\left(k_1^2(1 + \alpha) + k_2^2\right)\tilde{u}_1 + \partial^2\tilde{u}_1 \partial x_1^2 - \alpha k_1k_2\tilde{u}_2 - ik_1\partial\tilde{u}_2 \partial x_3 &= \\
- \frac{F}{2\pi\mu}\exp(ik_1\xi + ik_2\xi_2)\delta(x_3 - \xi_3) &= \\
- \alpha k_1k_2\tilde{u}_1 - \left(k_1^2 + k_2^2(1 + \alpha)\right)\tilde{u}_2 + \partial^2\tilde{u}_2 \partial x_3^2 - ik_2\partial\tilde{u}_3 \partial x_3 &= \\
- \frac{F}{2\pi\mu}\exp(ik_1\xi + ik_2\xi_2)\delta(x_3 - \xi_3) &= \\
- ik_1\partial\tilde{u}_1 \partial x_3 - ik_2\partial\tilde{u}_2 \partial x_3 - \left(k_1^2 + k_2^2\right)\tilde{u}_3 + (1 + \alpha)\partial^2\tilde{u}_3 \partial x_3^2 &= \\
- \frac{F}{2\pi\mu}\exp(ik_1\xi + ik_2\xi_2)\delta(x_3 - \xi_3)
\end{align*}
\]

(4)

where \(\alpha = 1/(1 - 2\nu)\) is introduced.

The solution of Eq. (4) is \(\tilde{u}_i = \exp(s x_i)\), where \(s\) values should be determined. Substitution into Eq. (4) with \(F_i = 0\) (homogeneous system) yields the characteristic equation for \(s\):
\[
-\left(k_1^2 + k_2^2 - s^2\right)(1 + \alpha) = 0.
\]

(5)

Eq. (5) has thrice degenerated roots \(s = \pm k\), where \(k = \sqrt{k_1^2 + k_2^2}\) is the module of the vector \(\mathbf{k}\). After the simple, but cumbersome transformations one can find the general homogeneous solution of Eq. (4) as
\[
\begin{align*}
\tilde{u}_1^h(k_1, k_2, x_3) &= \left(C_{10} + ik_1 x_3 C_{31}\right) \exp(-k x_3) + \left(C_{11} + ik_1 x_3 C_{33}\right) \exp(k x_3), \\
\tilde{u}_2^h(k_1, k_2, x_3) &= \left(C_{20} + ik_2 x_3 C_{31}\right) \exp(-k x_3) + \left(C_{21} + ik_2 x_3 C_{33}\right) \exp(k x_3), \\
\tilde{u}_3^h(k_1, k_2, x_3) &= \\
&= \left(-\frac{i}{k} C_{10} - \frac{k}{k} C_{20} + (3 - 4\nu)C_{31} + k x_3 C_{31}\right) \times
\end{align*}
\]
\[
\times \exp(-k x_3) + \\
+ \left(i \frac{k}{k} C_{11} + \frac{k}{k} C_{21} + (3 - 4\nu)C_{33} - k x_3 C_{33}\right) \exp(k x_3).
\]

(6)

Note, that the equality \(1 + 2/\alpha = 3 - 4\nu\) was used in Eqs. (6)-(8).

To complement the general solution, we seek the particular solution \(u_i^p(x)\) of the inhomogeneous Eqs. (4). One of the simplest is the solution for the homogeneous space \(u_i^p(x)\), since Eq. (1) is reduced to the system of algebraic equations when using the full 3D-Fourier transformation. Its solution has the form:
\[
\sigma_{ij}(\mathbf{k}) = \tilde{G}_{ij}^p(\mathbf{k}) F_j \exp(k \mathbf{k} \cdot \mathbf{x}).
\]

\[
\tilde{G}_{ij}^p(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \left(\begin{array}{c}
\frac{\partial \zeta_j}{\partial \zeta_i} - \frac{1}{k^2} k_i k_j
\end{array}\right).
\]

The inhomogeneous solution (9) corresponds to the well-known Fourier image of Green’s tensor for infinite homogeneous isotropic media (see e.g. Ref. [8]). Looking for solution of the system, confined in \(x_1\)-direction, it is convenient to transform (9) to coordinate representation on \(x_3\). Simple integration gives:
\[
\tilde{u}_i^p(k_1, k_2, x_3) = \\
= \tilde{G}_{ij}^p(k_1, k_2, x_3 - \xi_3) F_j \exp(ik_1\xi_1 + ik_2\xi_2),
\]

(10)

where
\[
\begin{align*}
\tilde{G}_{11}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[1 - \frac{k^2}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11a)

\[
\begin{align*}
\tilde{G}_{12}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[\frac{k}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11b)

\[
\begin{align*}
\tilde{G}_{13}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[1 - \frac{k^2}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11c)

\[
\begin{align*}
\tilde{G}_{22}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[\frac{k}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11d)

\[
\begin{align*}
\tilde{G}_{23}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[\frac{k}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11e)

\[
\begin{align*}
\tilde{G}_{33}^p(k_1, k_2, x_3 - \xi_3) &= \\
&= \frac{1}{4\pi\mu} \exp(-k x_3 - \xi_3) \left[\frac{k}{4(1 - \nu)k^2}\right],
\end{align*}
\]

(11f)

and \(\mu = \gamma/(2(1 + \nu))\).

The general solution of the chosen elastic problem should satisfy the boundary conditions at the rigid substrate is \(u_i(x_3 = h) = 0\) or \(u_i(x_3 = h)\) and \(\sigma_{3i}(x_3 = h)\) are continuous for the matched substrate; also \(\sigma_{3i}(x_3 = 0) = 0\) at free upper surface. Keeping in mind the Hook law \(\sigma_{ij} = c_{ijkl} u_{kl}\), where the strain
For the case 0332111 function is the solution for the matched substrate case. Should be solved allowing for the partial solution

\[
\begin{align*}
\sigma_{33} &= \frac{Y}{(1+v)(1-2v)}(u_{33} + v(u_{11} + u_{22})), \\
\sigma_{31} &= \frac{Y}{(1+v)}u_{13}, \quad \sigma_{32} = \frac{Y}{(1+v)}u_{23}.
\end{align*}
\]

For the rigid substrate case, the boundary conditions for \( \tilde{u}_i (k_1, k_2, x_3) = \tilde{u}_i^h(k_1, k_2, x_3) + \tilde{u}_i^p(k_1, k_2, x_3) \) have the form:

\[
\begin{align*}
&(1-v) \frac{\partial \tilde{u}_i^h}{\partial x_3} - iv(k_1 \tilde{u}_1 + k_2 \tilde{u}_2) = 0, \quad \text{at } x_3 = 0, \\
&(\frac{\partial \tilde{u}_1^h}{\partial x_3} - ik_1 \tilde{u}_1) |_{x_3=0} = 0, \quad \frac{\partial \tilde{u}_2^h}{\partial x_3} - ik_2 \tilde{u}_2 |_{x_3=0} = 0, \\
&\tilde{u}_1 |_{x_3=0} = 0, \quad \tilde{u}_2 |_{x_3=0} = 0, \quad \tilde{u}_3 |_{x_3=0} = 0.
\end{align*}
\]

Six constants \( C_j \) should be expressed via \( F_j \) from Eqs. (12). For the matched substrate only the first row of Eqs. (12) should be used.

(1) First step. Let us find the Green function \( \tilde{G}_{ij}^h(k_1, k_2, x_3 - \xi_3) \) of the semi-space (\( h \to \infty \)). The function is the solution for the matched substrate case. For the case \( C_{11} = C_{21} = C_{33} = 0 \) and then Eqs. (12) should be solved allowing for the partial solution \( \tilde{u}_i^p(k_1, k_2, 0) = \tilde{u}_i^h(k_1, k_2, 0) \). After cumbersome algebraic transformations one derives:

\[
\begin{align*}
\tilde{u}_i^h(k_1, k_2, x_3) &= \tilde{G}_i^h(k_1, k_2, x_3, \xi_3) F_i^h, \quad \text{exp}(ik_1 \xi_1 + ik_2 \xi_2).
\end{align*}
\]

Where

\[
\begin{align*}
\tilde{G}_{11}^h(k_1, k_2, x_3, \xi_3) &= \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)} \\
&\times \left( \frac{-k^2 k (x_3 + \xi_3) (3 - 4v) + 2k^2 (2-2v + k_{x_3}^2 x_3 + k_{11}^2 (l-8(1-v)v))}{16\mu k^3(1-v)} \right) + \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)} \\
\tilde{G}_{21}^h(k_1, k_2, x_3, \xi_3) &= \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)} \\
&\times k_1 k_2 \frac{2k^2 x_3 \xi_3 - k (x_3 + \xi_3) (3 - 4v) + 1 + 8(1-v)v}{16\mu k^3(1-v)} + \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)} \\
\tilde{G}_{31}^h(k_1, k_2, x_3, \xi_3) &= \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)} \\
&\times k_1 k_2 \frac{2k^2 x_3 \xi_3 + k (x_3 + \xi_3) (3 - 4v) + 1 + 4(1-v)(1-2v)}{16\mu k^3(1-v)} + \frac{\exp(-k(x_3 + \xi_3)}{16\mu k^3(1-v)}.
\end{align*}
\]
where \( k = \sqrt{k_1^2 + k_2^2} \). Note that

\[
\tilde{G}_{21}^i(k_1,k_2,x_3,z_3) = \tilde{G}_{12}^i(k_1,k_2,x_3,z_3),
\]

\[
\tilde{G}_{22}^i(k_1,k_2,x_3,z_3) = \tilde{G}_{11}^i(k_1,k_2,x_3,z_3),
\]

\[
\tilde{G}_{32}^i(k_1,k_2,x_3,z_3) = \tilde{G}_{31}^i(k_1,k_2,x_3,z_3)
\]

as expected.

(II) Second step. Using Eq. (14) as the partial solution \( \tilde{u}^p_i(k_1,k_2,x_3) = \tilde{u}_i^p(k_1,k_2,x_3) \), let us find the surface vertical displacement \( \tilde{u}_i^p(k_1,k_2,0) \) for the film of the thickness \( h \). Here \( \tilde{u}_i^p(k_1,k_2,0) \) should be found from Eqs. (12), namely after cumbersome algebraic transformations we derived that

\[
\tilde{u}_i^p(k_1,k_2,0) = \tilde{G}_{ij}^p(k_1,k_2,z_3)F_j \exp(ik_1z_1 + ik_2z_2).
\]

(15)

Where the elastic Green function \( \tilde{G}_{ij}^p(k_1,k_2,z_3) \) for the film on a rigid substrate has the form:

\[
\tilde{G}_{ij}^p(k_1,k_2,z_3) = \left( \tilde{G}_{ij}^p(k_1,k_2,0,z_3) - \tilde{G}_{ij}^p(k_1,k_2,h,z_3) \phi_1(k,h,v) + \left( \tilde{G}_{ij}^p(k_1,k_2,h,z_3) + k_i \tilde{G}_{ij}^p(k_1,k_2,h,z_3) \right) \phi_1(k,h,v) \right).
\]

(16)

\[
\phi_1(k,h,v) = \frac{4(1 - v) \exp(-kh)(2v + k - 2h) \exp((2v + k + 2h))}{(3 - 4v) \exp(-k(2v + k + 2h)) + 2(1 + 4(1 - v)(1 - 2v) + 2k^2h^2)}.
\]

(17a)

\[
\phi_1(k,h,v) = \frac{4(1 - v) \exp(-kh)(1 - 2v + k) \exp(k(1 - 2v - k))}{k((3 - 4v) \exp(-2k(h) + 2k(h) + 2(1 + 4(1 - v)(1 - 2v) + 2k^2h^2))}
\]

(17b)

Here \( k = \sqrt{k_1^2 + k_2^2} \), \( v \) is the Poisson ratio. Note that \( \tilde{G}_{ij}^p(k_1,k_2,0 < z_3 < h) = 0 \) at \( h = 0 \) as it should be expected. For the film on the matched substrate \( \phi_1(k,h,v) = 0 \) and \( \phi_1(k,h,v) = 0 \).

3. Resolution function and electric field calculations for thin piezoelectric films

The phenomenological resolution function theory for PFM based on linear imaging theory has been introduced in Ref. [9], where the resolution function and the effect of lock-in on resolution have been determined experimentally, and later on theoretically considered in Ref. [5] for the semi-infinite case.

Let us consider the case when the film dielectric and piezoelectric properties differ from bulk or substrate ones. In this case, the strain piezoelectric coefficient \( d_{ij}^S(x_1,x_2) \) is dependent on the depth \( x_3 \) as follows:

\[
d_{ij}^S(x_1,x_2,x_3) = \begin{cases} 
  d_{ij}^S(x_1,x_2), & 0 \leq x_3 \leq h \\
  0, & h < x_3 < \infty
\end{cases}
\]

(18)

Here, \( d_{ij}^S(x_1,x_2) \) are the film piezoelectric effect tensor components.

The surface piezoresponse below the tip \((x_3 = 0)\) is given by the convolution of piezoelectric coefficients \( d_{ij} \) with the surface and bulk components of the resolution function [9]:

\[
\tilde{u}_i^S(x_1,x_2,0) = \int_{-\infty}^{x_1} \int_{-\infty}^{x_2} W_{ijkl}^S(x_1 - \xi_1, x_2 - \xi_2)d_{ij}^S(x_1 - \xi_1, x_2 - \xi_2).
\]

(19)

The film resolution function [6] components \( W_{ijkl}^S \) are introduced as

\[
W_{ijkl}^S(\xi_1,\xi_2) = \int_0^h d\xi_3 \frac{\partial G_{ij}^f(\xi_1,\xi_2,\xi_3)}{\partial \xi_3} E_k(\xi_1,\xi_2,\xi_3).
\]

(20)

\( E_k(x) \) is the ac electric field distribution produced by the probe.

Hereafter the effective point charge model [10, 11] is used for electric fields description in the immediate vicinity of the tip-surface junction. Within the framework of the model, the charge value \( Q \) and its surface separation \( d \) are selected so that corresponding isopotential surface reproduces the tip radius of curvature in the contact point \( R_0 \) (or contact radius for flattened tip) and potential \( U \) (see Fig. 1). For piezoresponse modeling, the electric field structure can be represented by the point charge model in which the effective charge value \( Q \) is equal to the product of tip capacitance \( C_l(h) \) on applied voltage \( Q(h) = C_l(h)U \).

The electric field potentials \( \varphi_{electric}(r) \) created by the point charge \( Q \) localized in ambient in the point \( r_0 = (0,0,-d) \) outside the layer (film) \( 0 \leq x_3 \leq h \) filled by transversely isotropic dielectric with \( \varepsilon_{11} = \varepsilon_{22} \neq \varepsilon_{33} \) could be found from the boundary problem:
\[ \Delta \varphi_e (r) = - \frac{Q}{\varepsilon_0 \varepsilon_e} \delta(x_1, x_2, x_3 + d), \quad x_3 \leq 0, \]
\[ \varepsilon_{11} \Delta \varphi_1 (r) + \varepsilon_{33} \frac{\partial^2 \varphi_1}{\partial x_3^2} = 0, \quad 0 \leq x_3 \leq h, \]
\[ \varepsilon_{11} \Delta \varphi_1 (r) + \varepsilon_{33} \frac{\partial^2 \varphi_1}{\partial x_3^2} = 0, \quad x_3 \geq h, \]
\[ \varphi_e (x_3 = 0) = \varphi_1 (x_3 = 0), \left( \varepsilon_e \frac{\partial \varphi_e}{\partial x_3} - \varepsilon_{33} \frac{\partial \varphi_1}{\partial x_3} \right)_{x_3 = 0} = 0, \]
\[ \varphi_1 (x_3 = h) = \varphi_3 (x_3 = h), \left( \varepsilon_{11} \frac{\partial \varphi_1}{\partial x_3} - \varepsilon_{33} \frac{\partial \varphi_3}{\partial x_3} \right)_{x_3 = h} = 0. \]

(21)

Note, that \( \varphi_1 (x_3 = h) = 0 \) for a conductive substrate. The solution of Eq. (21) can be found with the help of Hankel integral transformation. Inside the film \( 0 \leq x_3 \leq h \), the Fourier representation of the electric field \( \vec{E}_f (k_1, k_2, x_3) \) acquires the form

\[ \vec{E}_{1,2} (k_1, k_2, x_3) = i k_{1,2} \frac{Q}{2 \pi \varepsilon_0} \times \]

\[ \left( \kappa_+ + \kappa \right) \exp \left( - \frac{k d - k x_3}{\gamma} \right) - \left( \kappa_+ - \kappa \right) \exp \left( - \frac{k d - k x_3}{\gamma} \right), \]

\[ \times \frac{1}{k} \left( \left( \kappa_+ + \kappa \right) \left( \varepsilon_e + \kappa \right) - \left( \kappa_+ - \kappa \right) \left( \varepsilon_e - \kappa \right) \exp \left( - \frac{2 h - x_3}{\gamma} \right) \right), \]

\[ \vec{E}_3 (k_1, k_2, x_3) = \frac{Q}{2 \pi \varepsilon_0} \times \]

\[ \left( \kappa_+ + \kappa \right) \exp \left( - \frac{k d - k x_3}{\gamma} \right) + \left( \kappa_+ - \kappa \right) \exp \left( - \frac{k d - k x_3}{\gamma} \right), \]

\[ \times \gamma \left( \left( \kappa_+ + \kappa \right) \left( \varepsilon_e + \kappa \right) - \left( \kappa_+ - \kappa \right) \left( \varepsilon_e - \kappa \right) \exp \left( - \frac{2 h - x_3}{\gamma} \right) \right). \]

(22)

Here \( \varepsilon_e \) is the dielectric constant of the ambient, \( \kappa = \sqrt{\varepsilon_33 \varepsilon_{11}} \) is effective dielectric constant, \( \gamma = \sqrt{\varepsilon_33 / \varepsilon_{11}} \) is the dielectric anisotropy factor of the film, \( \kappa_b = \sqrt{\varepsilon_33 / \varepsilon_{11}} \) is effective dielectric constant of the substrate; \( -d \) is \( x_3 \) coordinate of the effective point charge \( Q \). Usually \( d \sim 1 - 100 \) nm.

For the conductive disk of radius \( R_0 \) representing flattened tip-surface contact area, the effective charge \( Q(h) = C_{disk} (h) U \). Calculations performed in Ref. [6] lead to the probe tip effective capacity \( C_{disk} (h) = 4 \pi \varepsilon_0 (\varepsilon_e + \kappa) R_0 / \psi (h, d) \), where the function

\[ \psi (h, d) = \left( \sum_{n=0}^{\infty} \chi^n \left( \frac{\gamma d}{\gamma d + 2 \ln \left( \frac{\kappa_b + \kappa}{\kappa_b + \kappa} \right) \gamma d + 2 h (n + 1) \right) \right)^{-1}, \]

and the parameter \( \chi = \frac{\kappa_b - \kappa}{\kappa_b + \kappa} \). The corresponding effective distance \( d = 2 R_0 / \pi \), i.e. \( d \) is almost independent on the film thickness \( h \).

For the spherical tip with curvature \( R_0 \) in point contact with film surface, the effective charge \( Q(h) = C_{sph} (h) U \). We obtained the probe tip capacity \( C_{sph} (h) = 4 \pi \varepsilon_0 e_0 R_0 \kappa + \kappa / \kappa - e_0 \ln \left( \frac{\varepsilon_e + \kappa}{2 \kappa - e_0} \right) \times \]

\[ \times \left( 1 + \gamma \right) R_0 / h \left( \kappa_e - \kappa \right)^2 \right) \ln \left( \frac{\varepsilon_e + \kappa}{2 \kappa - e_0} \right) \]

and effective distance \( d \approx 2 e_0 R_0 \times \ln \left( \left( \kappa_e + \kappa \right) / \left( \kappa_e - \kappa \right) \right) \) for the film thickness \( h \gtrsim 0.1 R_0 \) in the actual range of high dielectric constants \( \kappa_e > 1 \) and \( 1 \leq e_0 \lesssim 80 \) [6].

For the considered case when a piezoelectric layer is inhomogeneous in the transverse directions \( \{x_1, x_2\} \) (e.g. it is divided into polar regions or posses domain structure with different piezoelectric tensor values and signs \( d_{ij} (x_1, x_2) \), the resolution function components \( W_{ij} (q) \) allow approximate calculation of the piezoresponse from those structures, which Fourier image \( \vec{d}_{ij} (q) \) exists in usual (e.g. domain stripes, rings etc.) or generalized (infinite plane domain wall) sense. Being more rigorous, one should use the Fourier image of tensorial object transfer function components \( \vec{W}_{ij} (q) \), since the Fourier transform of film vertical piezoresponse \( \vec{d}_{ij} (q) \) over transverse coordinates \( \{x_1, x_2\} \) is

\[ \vec{d}_{ij} (q) = \vec{W}_{ij} (q) \vec{d}_{ij} (q) + \vec{W}_{ij} (q) \vec{d}_{ij} (q) + \vec{W}_{ij} (q) \vec{d}_{ij} (q), \]

(23)

where \( \vec{d}_{ij} (q) = \int \vec{d}_{ij} (x) e^{i q x} / dx \) is the Fourier transforms of effective vertical piezoresponse \( d_{ij} (x = 0) \); the Voight notation is used. Object transfer function component \( \vec{W}_{ij} (q) \) spectrum dependent on wavenumber absolute value \( q = \sqrt{q_1^2 + q_2^2} \) is shown in Fig. 2a-c for various film thicknesses \( h \).

In most cases, the component \( \vec{W}_{ij} (q) \) corresponding to the piezoelectric constant \( d_{ij} \) provides the dominant (>50 %) contribution to the overall signal [5]. The two-point resolution \( r_{min} \) in PFM experiments is determined by the inverse halwidth of \( \vec{W}_{ij} (q) \). The dependence of corresponding two-point resolution \( r_{min} \) on \( h/d \) for different values of anisotropy \( \gamma \) is shown in Fig. 2d. It is clear that the information limit increases with the film thickness decrease because of \( r_{min} \) decrease. The dependence of 180°-periodic domain...
Fig. 2. (a, b, c) Object transfer function components $\bar{W}_{ij}^{(q)}$ spectrum for anisotropy $\gamma = 1$, permittivity $\kappa = 500$ and relative thickness $h/d = 0.3, 1, 3, 10$ (curves 1, 2, 3, 4); substrate permittivity $\kappa_b = 10$, ambient dielectric constant $\varepsilon_r = 1$. (d) The dependence of corresponding two-point resolution $r_{\min}/d$ on $h/d$ for different values of anisotropy $\gamma = 0.25, 0.5, 1, 3$ (curves 1, 2, 3, 4).

Fig. 3. (a) The dependence of 180°-periodic domain structure resolution $a_{\min}$ via PbTiO$_3$ film thickness $h$ on a rigid substrate for the effective distance $d = 10$ nm. (b) Information limit defined as a minimal domain stripes period $a$ calculated from the condition $\{d_W^{(a)}(a, h)\} = \text{noise level}$ for the PbTiO$_3$ film of the thickness $h$ on a rigid substrate for the typical noise level 1 pm/V and different tip-surface contact radii $R_0 = 3, 6, 9$ nm (effective distance $d = 2R_0/\pi$). (b) PbTiO$_3$ material parameters $\nu = 0.35$, $\kappa = 121, \gamma = 0.87$, $d_{15}^3 = 117$, $d_{15}^3 = 61$, $d_{31}^3 = -25$ pm/V, substrate permittivity $\kappa_b = 5$, ambient permittivity $\varepsilon_r = 1$. 

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structure resolution via the film thickness $h$ and corresponding information limit defined as minimal domain stripes period $a_{\text{min}}$ calculated from the condition $\max \left\{ d_{\text{eff}}(a,h) \right\} = \text{noise level}$ is shown in Fig. 3 for the PbTiO$_3$ film on a rigid substrate.

4. Conclusion

The elastic Green function and resolution function in Piezoresponse Force Microscopy (PFM) of piezoelectric film capped on the rigid substrate with different dielectric properties are derived.

The thickness dependence of resolution function of the thin piezoelectric films on rigid substrates is demonstrated: minimal lateral resolution (or higher information limit) is possible in thin films. However, the signal amplitude essentially decreases with film thickness decrease, eventually making the noise level relatively higher.

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