Multiscale model for atomic force microscope array mechanical behavior

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The author presents a first simplified two-scale model of the elastic structure of an atomic force microscope array. It can be used for rapid prototyping and for designing model based control loops. Its derivation is based on the concept of two-scale approximation. © 2007 American Institute of Physics. [DOI: 10.1063/1.2710001]

The atomic force microscopy (AFM) has been invented by Binnig and reported in Ref. 1. Since that time, many applications have emerged in various fields of sciences and technologies. The main limitations of the AFM devices are their low speed and reliability of operation. This may be improved by designing model based control, see, for instance, Ref. 2. Today, the technology has evolved towards fabrication of AFM arrays, see, e.g., Ref. 3, and model based control can also help to improve their efficiency. In this letter we present, for the first time, a simplified elastic AFM array model that can be used for control as well as for rapid prototyping. Its rigorous derivation is based on the mathematical concept of two-scale approximation, see Refs. 4–6, and will be reported in a forthcoming paper.

We consider a two-dimensional array of AFMs comprised of \( n_1 \) parallel elastic bases, oriented on the \( x_1 \) direction, and \( n_1 \) clamped elastic cantilevers per base. The cantilevers are equipped with a rigid tip. They are oriented in the \( x_2 \) direction and are distributed periodically along the bases, see Fig. 1. The characteristic size of a periodicity cell is denoted by \( e \). The length, the width, and the thickness of the bases are denoted by \( L_B, \varepsilon L_B, \) and \( a_B \). Those of the supple part and of the rigid part of the cantilevers are, respectively, \( \varepsilon L_F, \varepsilon L_R, \varepsilon L_W, \) and \( \varepsilon L_{\text{tip}} \), see Fig. 2 for the in-plane dimensions. The array is comprised of an isotropic homogeneous material with density \( \rho \) and Lamé constants \( \lambda, \mu \). It occupies the domain denoted by \( \Omega_p \) and is assumed to be thin enough for being modeled by the Love-Kirchhoff thin plate equation. For the sake of shortness, we consider only forces applied to the cantilever tips.

The domain \( \Omega_p \) is included in \( \Omega = \omega \times (-\ell, 0/2, \ell, 0/2) \) with section \( \omega = (0, L_1) \times (0, L_2) \) and decomposed in a set of \( n_1 \times n_2 \) cells of periodicity \( Y_i \) with size \( e \ell_1 \times e \ell_2 \times e \ell_3 \). In other words, \( \Omega_p = n_1 \ell_1, L_2 = n_2 \ell_2, \) and the multi-index \( i = (i_1, i_2) \) varies in \( \{1, \ldots, n_1\} \times \{1, \ldots, n_2\} \). We introduce the reference cell \( Y = \Omega_{\text{ref}} = (-\ell, 0/2, \ell, 0/2) \) deduced from the cells \( Y_i \) by a shift and a dilatation by \( 1/e \). Through the same shifts and dilatation, the intersections \( Y_i \cap \Omega_p \) are transformed into the array reference cell \( Y_p \subset Y \).

We denote by \( u^t(t,x) \) the transverse mechanical displacement solution of the Love-Kirchhoff thin plate equation in \( \Omega_p \) which is independent of \( x_3 \). Its two-scale approximation is defined through the three following steps where the time variable plays the role of a parameter.

1. The two-scale transform \( \hat{u}^p \) of \( u^p \) is a function of the variable macro \( \tilde{x} \in \omega \) and of the variable micro \( y \in Y_p \). It is defined by

\[
\hat{u}^p(t, \tilde{x}, y) = \sum_{i \in \{1, \ldots, n_1\} \times \{1, \ldots, n_2\}} \chi_Y(\tilde{x}, 0) u^p(t, x_i + ey),
\]

where \( x_i \) denotes the center of \( Y_i \).

2. The AFM size \( L_1 \times L_2 \) being frozen, we consider the geometry of the array as depending on the parameter \( e \). Thus, the two-scale transform \( \hat{u}^p \) is a function of \( e \) which is assumed to be sufficiently regular so that the expansion

\[
\hat{u}^p = u^A + O(e)
\]

holds, with \( u^A \) a function defined on \( \omega \times Y_p \) independent of \( e \).

3. Finally, the two-scale approximation of \( u^p \) is \( \bar{u}^p \) defined on \( \Omega_p \) by

\[
\bar{u}^p(t, \tilde{x}) = \sum_{i \in \{1, \ldots, n_1\} \times \{1, \ldots, n_2\}} \chi_Y(\tilde{x}, 0) u^A(t, x_i, (x_2 - x_{2i})/e)
\]

for a function \( u^A \) depending on \((t, x_1, x_2)\) only.

Now, we state the AFM array model, for one row, under the assumption that the displacement in each cantilever is constant in the \( x_1 \) direction and that the cantilevers are much thinner than the base or more precisely that \( a_B = \varepsilon (e/\ell_1)^{1/3} \). Since the array is not connected in the direction \( x_2 \), this variable plays the role of a parameter and can be ignored in the considered case. The forces applied to the tip of the \( i \)th cell are denoted by \( F_i \). For the sake of convenience, let us introduce the variable \( y^C_2 = y_2 - \ell_B + \ell_2/2 \) that vanishes at the junction between the base and the cantilever in \( Y_p \). It appears that \( u^A \) is independent of \( y_2 \) in the base, so the model equations are expressed in the rectangular domain \((x_1, y^C_2) \in (0, L_1) \times (0, L_2 + L_{\text{tip}})\). The line \( y^C_2 = 0 \) corresponds to the base, the open rectangle \((0, L_1) \times (0, L_{\text{F}})\) represents the elastic part of the cantilevers, and \((0, L_1) \times (L_{\text{F}}, L_{\text{F}} + L_{\text{tip}})\) its rigid part. For \( t > 0 \) and \( x_1 \in (0, L_1) \),

\[
\rho^A \ddot{u}^A + R^A \dddot{u}^A _{x_1} + u^A + \ell_B R^C \dddot{u}^A _{y^C_2} u^A = 0
\]

for \( y^C_2 = 0 \) and

\[
\rho^A \ddot{u}^A + R^C \dddot{u}^A _{y^C_2} u^A = 0
\]

for \( y^C_2 \in (0, L_{\text{F}}) \). The boundary conditions are \( u^A = \partial_1 u^A = 0 \) for \((x_1, y^C_2) \in (0, L_1) \times \{0\}\), \( \partial_2 u^A = 0 \) for \((x_1, y^C_2) \in (0, L_1) \times \{L_2 + L_{\text{tip}}\}\), and

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The model is modified by setting \( Q \) to \( -\lambda^A \). They constitute an infinite sequence and can be written under the form \( \lambda_{k}^{A} = R^{C} \lambda_{k}^{C} / (\rho^{F} L_{F}^{2}) \) and \( \psi_{k_{1},k_{2}}(x_{1},y_{2}) = \psi_{k_{1}}(x_{1}/L_{1}) \psi_{k_{2}}(y_{2}/L_{F}) \) for \((k_{1},k_{2}) \in \mathbb{N} \times \mathbb{N}, \) where \((\lambda_{k}^{C},\varphi_{k}^{C})\) is the solution of the spectral problem

\[
\varphi^{B_{m}}(0,1),
\]

\[
\varphi^{B} = 0 \text{ at } (0,1),
\]

and for each \( \lambda^{B}, (\lambda^{C},\varphi^{C}) \) is the solution of the spectral problem

\[
\varphi^{C_{m'}} = \lambda^{C} \varphi^{C} \text{ in } (0,1),
\]

\[
\varphi^{C_{1}}(0) = 0,
\]

\[
q^{1} \varphi^{C_{m}}(0) = (q^{0} \lambda^{C} - \lambda^{B}) \varphi^{C}(0),
\]

with \( Q^{F} = (\varepsilon/2a_{F}L_{F}^{2})Q_{S}S_{Q}, \) \( S_{Q} = (0,1) \), \( q^{0} = L_{F}^{2}R^{C} (\rho^{F} L_{F}^{2}), \) and \( q^{1} = L_{F}^{2}R^{C} \partial_{y}L_{F}/(L_{F}^{3}R_{M}^{2}). \) For \( \lambda^{B} \) large enough, \((\lambda^{C},\varphi^{C})\) are independent of \( \lambda^{B} \), so they may be indexed by the index \( k_{2} \) only. In our simulations, we have

\[
\begin{array}{cccccccccc}
\text{Tips} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
(\%a) & 8 & 9 & 11 & 12 & 100 & 13 & 12 & 11 & 1 & 0.9 \\
(\%b) & 1.2 & 0.5 & 0.3 & 0.2 & 100 & 0.2 & 0.3 & 0.5 & 1.2 & 0.9
\end{array}
\]

Remark: If the cantilevers are not equipped with a rigid part, the model must be modified by setting \( Q = 0. \)

For the model illustration, some simulations with a force oscillating at the first cantilever eigenfrequency and applied to the fifth tip (a) or to the fifth and sixth tips (b) have been conducted. The structure is isotropic and homogeneous, its volume mass is \( \rho = 2329 \text{ kg/m}^{3} \), and its Lamé coefficients are \( \lambda = 6.1 \times 10^{11} \text{ and } \mu = 5.2 \times 10^{11}. \) The other parameters are \( \varepsilon = 50 \mu m, \) \( \ell_{1} = 1, n_{1} = 10, n_{2} = 1, \) \( \ell_{B} = 0.333, a_{B} = \varepsilon/5 \text{ m}, \) \( \ell_{F} = \ell_{ip} = L_{ip} = 0.25, \) \( L_{F} = 0.833, \) \( a_{F} = \varepsilon/40 \text{ m}, \) and \( a_{tip} = \varepsilon/2 \text{ m}. \) The ratios of the maximum displacement of the ten tips to these of the excited tips [(a) the fifth tip and (b) the fifth and the sixth tips] are reported in Table I.

We denote by \((\lambda^{A},\varphi^{A})\) the solutions of the associated spectral problem which is derived from the above model by replacing \( u^{A} \) by \( \psi^{A} \) and \( \partial_{y}^{2} \) by \(-\lambda^{A}\). They constitute an infinite sequence and can be written under the form \( \lambda_{k_{1},k_{2}}^{A} = R^{C} \lambda_{k}^{C} / (\rho^{F} L_{F}^{2}) \) and \( \psi_{k_{1},k_{2}}(x_{1},y_{2}) = \psi_{k_{1}}(x_{1}/L_{1}) \psi_{k_{2}}(y_{2}/L_{F}) \) for \((k_{1},k_{2}) \in \mathbb{N} \times \mathbb{N}, \) where \((\lambda_{k}^{C},\varphi_{k}^{C})\) is the solution of the spectral problem

\[
\begin{align*}
\varphi^{B_{m'}}(0,1), \\
\varphi^{B} = 0 \text{ at } (0,1),
\end{align*}
\]

and for each \( \lambda^{B}, (\lambda^{C},\varphi^{C}) \) is the solution of the spectral problem

\[
\begin{align*}
\varphi^{C_{m'}} = \lambda^{C} \varphi^{C} \text{ in } (0,1), \\
\varphi^{C_{1}}(0) = 0,
\end{align*}
\]

\[
q^{1} \varphi^{C_{m}}(0) = (q^{0} \lambda^{C} - \lambda^{B}) \varphi^{C}(0),
\]

where \( \lambda_{k}^{C} = q^{0} \lambda^{C} / (\rho^{F} L_{F}^{2}) \) and \( \varphi_{k}^{C} = L_{F}^{2} \varphi^{C} / (L_{F}^{3} R_{M}^{2}). \) For \( \lambda^{B} \) large enough, \((\lambda^{C},\varphi^{C})\) are independent of \( \lambda^{B} \), so they may be indexed by the index \( k_{2} \) only. In our simulations, we have

\[
\begin{array}{cccccccccc}
\text{Tips} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
(\%a) & 8 & 9 & 11 & 12 & 100 & 13 & 12 & 11 & 1 & 0.9 \\
(\%b) & 1.2 & 0.5 & 0.3 & 0.2 & 100 & 0.2 & 0.3 & 0.5 & 1.2 & 0.9
\end{array}
\]
found that this was always the case. We denote by \((\lambda^p, \varphi^p)\) the solution of the spectral problem associated with a single clamped cantilever. It is governed by the same equation that Eq. (3), except that the last boundary condition is replaced by \(\varphi^p(0)=0\). The first graph of Fig. 3 represents the eigenvector \(\varphi_0^C\) and the others the superimposed images of the eigenvectors \(\varphi_{k_2}^C\) in solid line and of the eigenvectors \(\varphi_{k_2}^P\) in dashed line for \(k_2 = 1, \ldots, 3\). For \(k_2 \geq 1\), the modes \(\varphi_{k_2}^C\) and \(\varphi_{k_2}^P\) differ mainly by a constant that becomes smaller when \(k_2\) increases. The logarithm of the eigenvalues \(\lambda_{k_2}^A\) for \(k_2 = 0, \ldots, 8\) with markers “o” and \(\lambda_{k_2}^P\) for \(k_2 = 1, \ldots, 9\) with markers “+” is compared in Fig. 4. Finally, the eigenvectors \(\varphi_{k_1,k_2}^A\) for \((k_1,k_2) \in \{1,2\} \times \{0,1\}\) are displayed in Fig. 5.

The AFM array model presented here is extremely light, so it can be used for real time model based control of the array as well as for model based image processing. Further extensions of the models are also suitable to encompass electrostatic and thermal couplings.