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The Importance of Distributed Loading and Cantilever Angle in Piezo-Force Microscopy*

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Abstract. Piezo-force microscopy (PFM) is a variation of atomic force microscopy that is widely applied to investigate piezoelectric thin films at the nanometer scale. Curiously, PFM experiments are found to be remarkably sensitive to the position along the cantilever at which deflection is detected, complicating attempts to use this technique to quantify surface actuation and thereby measure the converse piezoelectric coefficient. A straightforward analytical theory is proposed that accounts for this observation by combining standard PFM analyses with subtleties of the typical AFM detection mechanism as well as the concept of distributed loading. Corresponding simulations of PFM measurements indicate that these experimental artifacts can even lead to an apparent inversion of the detected domain orientation. To better understand the importance of these effects, simulations are used to qualitatively map the theoretical PFM response for a wide range of typical experimental parameters, as well as the relative difference between these measurements and true piezoactuation.

Keywords: PFM, cantilever, piezoelectric, ferroelectric, AFM

Introduction

Piezo-force microscopy (PFM) was developed from Atomic Force Microscopy (AFM) to investigate the converse piezoelectric effect of piezoelectric materials. This technique is now widely implemented, especially to characterize thin film homogeneity, identify domain orientation, and determine various piezoelectric coefficients [1]. At its simplest, a periodic bias is applied between a rear electrode on a sample and a conducting AFM tip. This is assumed to cause local piezoactuation at the tip, which translates 100% to the end of the lever, which is ultimately detected by a focused laser reflected off of the end of the lever. The phase of the lever response with respect to the drive signal is thought to relate directly to the domain orientation. More sophisticated models accounting for long range interactions between the sample and the incorporated cantilever [2], as well as sample mechanics, have been reported [3]. However, several important details have been overlooked by the AFM community, each having profound influences on PFM measurements under certain circumstances as described below.

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Body

The first detail of consequence for PFM interpretation relates to the mechanics of the measurement; specifically, the tip always maintains contact with the sample. First recognized and qualitatively explained by Hong et al. [4], any long range loads acting on the lever must be considered as being applied over the entire lever surface, instead of merely at the AFM tip as is generally assumed (which is approximately correct for noncontact measurements only). Figure 1 sketches a PFM experiment, depicting these so called distributed loads due to capacitive and Coulombic forces between the lever and

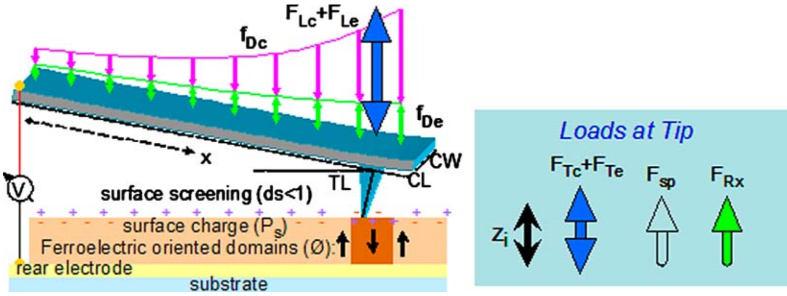

Fig. 1. Sketch of long range distributed loads, surface actuation, and tip loads acting on an integrated tip and cantilever during PFM.

sample (f_{Dc} and f_{De}, respectively). A localized force is still applied at the tip ($F_{Lc} + F_{Le}$) due to the distributed loads, but this is only $^3/_8$ of the integrated force that is usually assumed to act across the lever given a uniform load. Coulombic forces are attractive or repulsive depending on the orientation of the domain (surface charge) and the applied bias, whereas capacitive forces are always attractive.

Several other loads also act at the tip, including capacitive and Coulombic forces between the tip and sample ($F_{Tc} + F_{Te}$), the setpoint force maintained during the PFM experiment (F_{sp}), and the reaction load (F_{rx}, essentially the sample pushing back against all other locally applied loads). Finally, the surface itself moves (z_i) due to two effects: force dependent indentation (a relatively insignificant function of the sample mechanical properties for typical loads and biases [7]), and piezoactuation due to the bias locally applied by the tip and the domain orientation (Ø). Throughout this work, several simplifying assumptions have been made: the lever is not tilted with respect to the sample, lever motion occurs at frequencies far from resonance and thus obeys statics, the tip/sample indentation obeys Hertzian mechanics [5], forces from the sides of the tip are insignificant compared to the tip apex and lever surface, there is a 1 nm thick dead layer at the sample surface, the entire voltage (V) drops across the thin film and dead layer, a fraction of the surface charge (P_s) is screened by oppositely charged adsorbed species (ds), the piezoelectric film is assumed to have an 001 orientation and off-axis coefficients are ignored, and finally the oriention of all domains is the same direction except for those domains directly beneath the tip.

Several of these assumptions were relaxed elsewhere (lever tilt, surface dead layer thickness and dielectric constant, off-axis terms), but this did not qualitatively alter the results [7] and tremendously complicated the analytical description of the measured deflection. It is important to note, though, that for the case where domains are oriented randomly and are significantly smaller than the lever dimensions, the net effect of Coulombic interactions will be zero thereby diminishing the distributed loading influence. Nevertheless, a DC offset between tip and sample is likely due to work function differences and the surface potential of various domains, so the proposed PFM model still applies as capacitive forces will inevitably remain.

Based on these simplifying assumptions, Fig. 2(b) displays the theoretical true lever displacement for DC applied biases of +4, 0, and −4 Volts as described by Eqs. (1) and (2) [6] (where x is the position along the lever from the base). The capacitive and Coulombic terms are described in detail elsewhere [7]; also, piezoactuation is disregarded for now. Accounting for distributed loads clearly yields a dependence on the position at which the AFM deflection is detected (if the distributed load is ignored, the profiles for ±4 V will be essentially the same as for 0 V). In reality, though, most commercial AFM systems employ a beam bounce detector scheme (Fig. 2(a)) that does not sense displacement directly, but rather the lever angle (which can be linearly calibrated to displacement for the conditions of tip loading only). This angle is shown as a function of position in Fig. 2(c), calculated by taking the arctangent of the true displacements in Eq. (1) and Fig. 2(b). The corresponding signal measured by most commercial AFM's, calibrated for tip loading, is described by Eq. (3) and plotted in Fig. 2(d). This measured lever deflection is evidently even more sensitive to detection position than the true deflection (Fig. 2(b)), with a node at approximately 60% of the lever length.

$$\mathrm{def}_{\mathrm{true}}(x) = \left[\frac{x^2(x^2 - 4xCL + 6CL^2)}{8k_cCL^3}\right](\Psi) + \left[\frac{x^2(3CL - x)}{2k_cCL^3}\right]$$

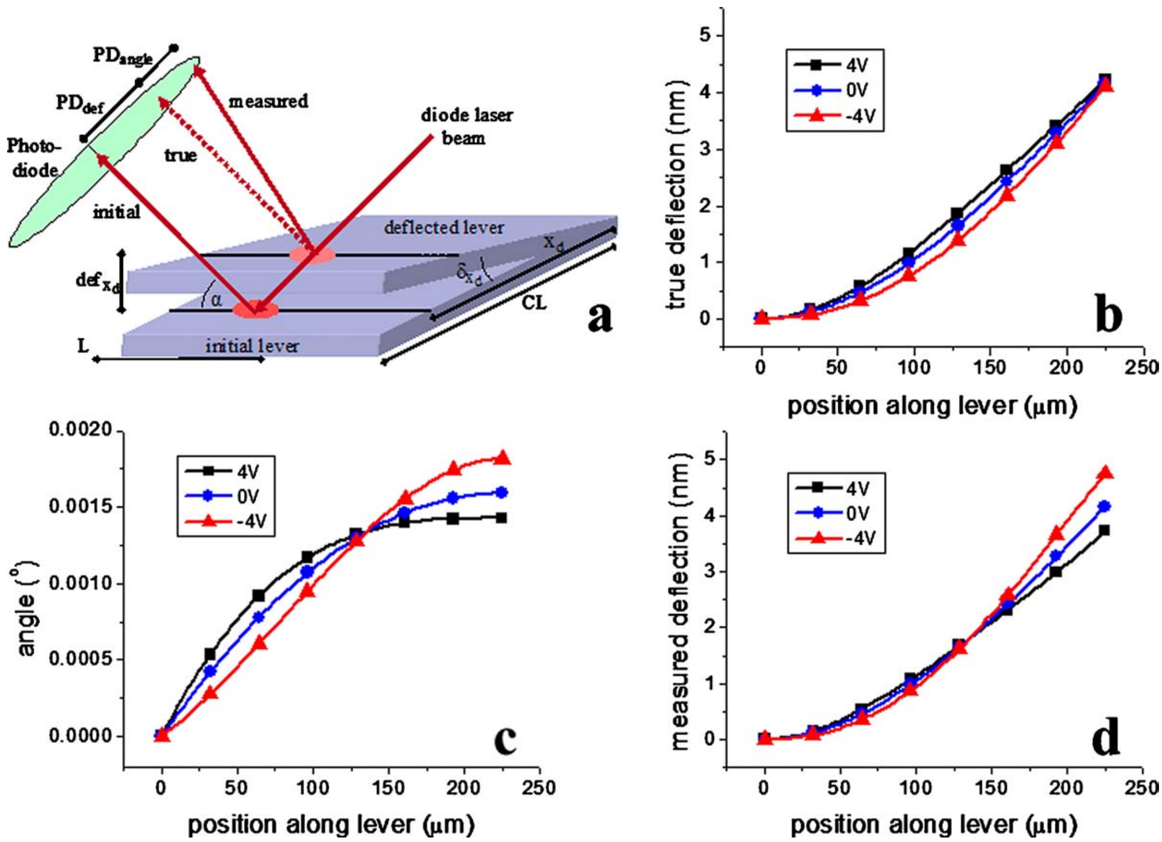

Fig. 2. Sketch of typical AFM sensitivity to angle (a), as well as the theoretical true deflection (b), angle (c), and measured deflection (d) along the lever.

$$\times \left(-\frac{3CL}{8}(\Psi) + F_{sp} + k_c z_i\right) \qquad (1)$$

$$\Psi = \left(f_{Dc_o} * V^2 + f_{De_o} * \phi * V\right) \quad \text{and}$$

$$V = V_{dc} + V_{ac}\sin\omega t \qquad (2)$$

$$\begin{aligned}\mathrm{def}_{\mathrm{meas}}(x) &= \left(\frac{x}{3}\right)\left(\frac{3CL-x}{2CL-x}\right)\left[\frac{\partial \mathrm{def}_{\mathrm{true}}(x)}{\partial x}\right]\\ &= \frac{1}{16k_cCL^3}\left(\frac{x}{3}\right)\left(\frac{3CL-x}{2CL-x}\right)\\ &\quad \times [(\Psi * x(8x^2 - 15xCL + 6CL^2))\\ &\quad + k_c z_i(24x)(2CL-x)] \qquad (3)\end{aligned}$$

Simulations of PFM measurements have been performed using this proposed theory, extended to calculate the 1st harmonic amplitude and phase for biases with both DC and AC components. Figure 3(a) presents the theoretical lever response, combined as amplitude*cos(phase), for the same case as in Fig. 2 but for an AC amplitude of 1 V with a DC offset of ±5 V (piezoactuation is still ignored). Figure 3(b) uses the same axes, but presents true experimental results obtained with an AFM with the tip in contact with a glass slide and integrated back electrode (the same configuration as Fig. 1, but the sample is a dielectric instead of a ferroelectric). The error bars represent standard deviations at each position for at least 10 amplitude and phase measurements of the biased tip and cantilever. The predicted and actual lever responses agree remarkably, including the position of the node as expected, evidencing the importance of the distributed load and lever angle. The same behavior has been observed with piezoelectric films as well [8].

Finally assuming a sample that is piezoelectric, the measured lever response for a wide range of independently varied experimental parameters has been simulated (Fig. 4(a)). For each data series, the following terms were held constant except for the parameter of interest (and used in the calculations

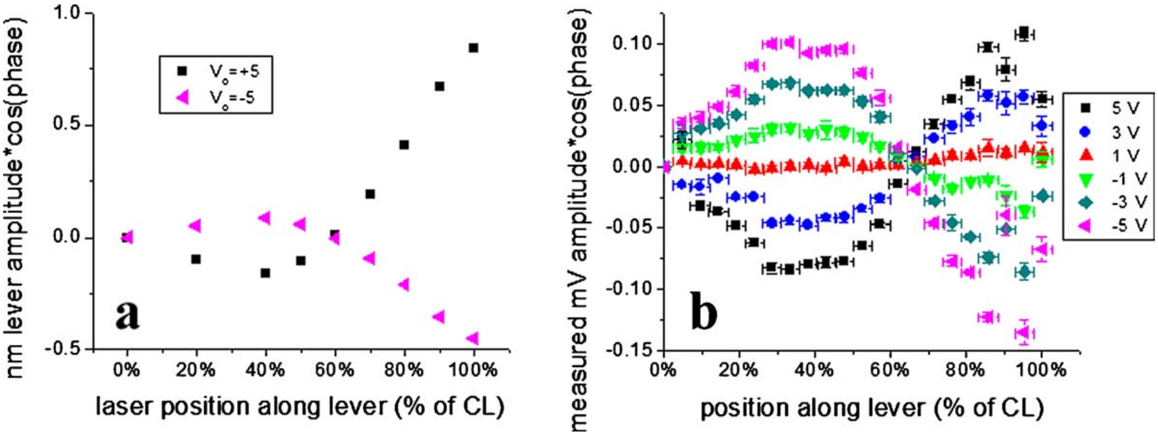

Fig. 3. Simulated (a) and experimental results (b) of the measured first harmonic response of a cantilever to periodic tip/lever biasing as a function of position along the lever and DC offset.

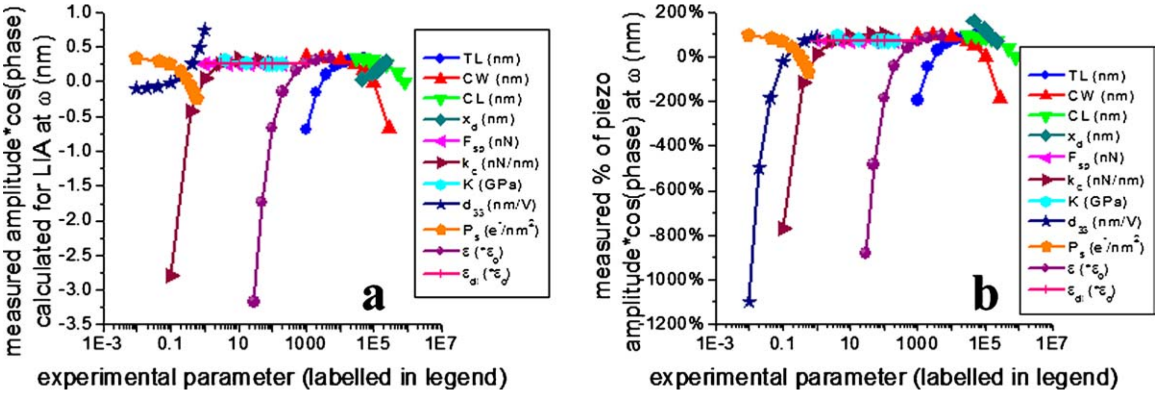

Fig. 4. Simulated measured PFM signal (a) and the proportion of that signal due to piezoactuation only (b).

described earlier unless otherwise noted): tip length (TL = 10,000 nm), lever width (CW = 28,000 nm), lever length (CL = 225,000 nm), detection position (x_d = 90% of CL), AFM setpoint force (F_{sp} = 10 nN), cantilever spring constant (k_c = 2.4 nN/nm), reduced modulus (K = 101 GPa), converse piezoelectric coefficient (d_{33} = 0.423 nm/V), surface charge (P_s = 0.15 C/m^2), surface charge screening (ds = 90%), film dielectric constant ($\varepsilon = 1000\varepsilon_o$), and dead layer dielectric constant ($\varepsilon = 30\varepsilon_o$). A DC bias of 0 volts was assumed for the tip, with a resulting tip-sample DC offset of ±50 mV due to the surface potential of oriented domains. Many other details could be included to be more quantitative, including variations in surface charge and potential due to back electrode influences, thin film texture and off axis piezoactuation terms, and even mechanical constraints within the film, but these are left for future work.

The significant dependence of PFM measured results predicted by Fig. 4(a) is especially troubling given that the true surface piezoactuation was held constant (±0.423 nm) for every single calculation except those of the data series d33 (proportional to $d_{33} * V * Ø$ as expected). But since d_{33} is generally the parameter of interest when performing PFM, the measured response relative to true piezoactuation only is presented in Fig. 4(b). For many typical conditions the ratio is negative, revealing that in addition to being incorrect quantitatively, the measured signal can also be out of phase with respect to the true local piezoactuation. These errors are influenced most by conditions such as low lever spring constants, short tips, diminishing film dielectric constants, variations in the converse piezoelectric coefficient, and increasing unscreened surface charges. Since these last three parameters are likely to vary spatially and simultaneously, and perhaps temporally, changes in the apparent amplitude or phase from a PFM map of a piezoelectric thin film are therefore difficult to interpret.

Based on these results, several exceptions can be inferred to allow quantitative measurements and mapping using PFM. The sample and lever should be shielded to minimize distributed Coulombic loads [9], and minimal DC offsets should be used to limit distributed capacitive effects. Measurements should be made at a fixed and known position along the lever, ideally at the node, to minimize measurement artifacts. Lastly, other techniques should be employed to ascertain whether mapped variations in the PFM response are related to independent or coupled changes in the dielectric constant, surface charge, and piezoelectric coefficients.

Conclusion

Several challenges are presented for the quantitative characterization of piezoelectric thin films using Piezoforce microscopy. First, PFM employs a fixed cantilever base and a sliding tip, leading to a different lever and tip response to DC or periodically applied biases than previously thought by the AFM community. Second, the measured lever response can differ dramatically, both in theory and experimentally, from the true response due to the angular sensitivity of typical AFM equipment and the corresponding strong influence of distributed loads. Incorporating these artifacts for the first time, an analytical PFM model is proposed that successfully predicts the experimentally confirmed sensitivity of the PFM response to the detection position along the lever. Even more important, the measured response during PFM has been simulated for a wide range of common experimental parameters and found to seldom agree with the true surface piezoactuation. The measured orientation of domains beneath the tip can even be the inverse of the actual orientation. For quantitative PFM results two guidelines are clear: the surface potential and charge for both sample and lever must be minimized by shielding, and the position along the lever at which deflection is measured must be accounted for.

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