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1 **EULER-BERNOULLI THEORY ACCURATELY PREDICTS ATOMIC FORCE**
2 **MICROSCOPE CANTILEVER SHAPE DURING NON-EQUILIBRIUM SNAP-TO-**
3 **CONTACT MOTION**

4
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ABSTRACT

We prove that the Euler-Bernoulli elastic beam theory can be reliably used to describe the dynamics of an atomic force microscope cantilever during the far from equilibrium snap-to-contact event. In conventional atomic force microscope operation, force-separation curves are obtained by post-processing voltage versus time traces produced by measuring one point on the cantilever close to the hanging end. In this article, we assess the validity of the Euler-Bernoulli equation during the snap-to-contact event. The assessment is based on a direct comparison between experiment and theory. The experiment uses Doppler vibrometry to measure displacement versus time for many points along the long axis of the cantilever. The theoretical algorithm is based on a solution of the Euler-Bernoulli equation to obtain the full shape of the cantilever as a function of time. The algorithm uses as boundary conditions, experimentally obtained information only near the hanging end of the cantilever. The solution is obtained in a manner that takes into account non-equilibrium motion. Within experimental error, the theory agrees with experiment indicating that the Euler-Bernoulli theory is appropriate to predict the cantilever kinematics during snap-to-contact. Since forces on the tip can be obtained from the instantaneous shape of the cantilever, this work should allow for computation of tip-sample forces during the snap-to-contact event from a conventional force-distance measured input.

Key Words: AFM, atomic force microscopy, far from equilibrium AFM cantilever, force distance curve

47 INTRODUCTION

48

49 The central hypothesis of this paper is that the Euler-Bernoulli equation provides a valid
50 model by which the kinematics of an AFM cantilever can be obtained during the far-from-
51 equilibrium snap-to-contact event. This event is often purposely avoided to stay within the
52 regime in which harmonic analysis can be performed. However, the snap-to-contact presents a
53 unique opportunity to test samples at closest approach. It allows for optimal sensitivity to
54 rapidly changing surface forces, allows for optimal lateral resolution because the situation can be
55 analyzed at arbitrarily small tip-sample separation, and provides a method for obtaining these
56 results with a simple experimental setup that requires no lock-in amplifiers. Motivated by these
57 observations, we sought to determine if a conventional AFM that provides cantilever
58 displacement measures only at the hanging end, can be used in conjunction with the Euler-
59 Bernoulli equation to obtain the full cantilever kinematics. Since forces on the tip can be
60 obtained from the instantaneous shape of the cantilever,[1] this work should allow for
61 computation of tip-sample forces during the snap-to-contact event from a conventional force-
62 distance measured input.

63 Atomic force microscopy is capable of generating topographical and surface
64 spectroscopic information even at length scales below a nanometer. To obtain this information
65 reliably and quantitatively, it is necessary for the user to know what forces the cantilever
66 experiences at each instant of operation. Thus, the mathematical prediction of the kinematics of
67 the cantilever sensor plays a central role in defining the output accuracy of the force
68 reconstruction algorithm in atomic force microscopy. To date, this description is well tested for
69 quasi-static operation and for operation where the cantilever is driven in one or more of its
70 normal modes. In this article, we study the validity of the assumption that the cantilever's
71 kinematics can be obtained from the Euler-Bernoulli equation [2-4] even under the specific
72 conditions of non-equilibrium motion and non-linear external forces. These common
73 circumstances exist during the snap-to-contact event, when the atomic force microscope tip
74 experiences the last few nanometers of travel before impacting the surface.

75 While the non-equilibrium motion mentioned above is not present in multifrequency
76 operation,[5, 6] the newer commercially available techniques involving off-resonance motion of
77 the lever as accomplished with peak force mode and fast force mapping do contain non-
78 equilibrium motion[7]. These methods take the lever through a single stroke similar to the slow
79 force-separation curve dealt with in the present paper.

80 In the past three decades, atomic force microscopy[8] has produced images of soft and
81 hard matter surfaces with submicron, even nanometer resolution [9-18]. Nevertheless,
82 considering its recent centrality in the imaging of materials surfaces and the vast technical
83 improvements regarding data collection speed and resolution, [5, 19] the technique is not yet
84 completely quantitative. This is due to a large extent both to the lack of full information of the
85 interaction forces between the sample and the tip, and to an unavoidable mismatch between the
86 mathematically modeled cantilever and the real one.

87 Since the inception of atomic force microscopy, imaging has been based on monitoring
88 variations of experimental parameters as the cantilever/tip sensor moves from one pixel to the
89 next. In the conventional experimental implementation of the image reconstruction, an optic
90 lever system is used to measure the position of the tip or, more accurately, the slope of the
91 cantilever at the tip's position. A photodetector output voltage is rapidly recorded at each pixel
92 while the tip moves up and down as a consequence of topographical and chemical variations on

93 the surface. Thus, by looking at all pixels within the field of view, a surface image can be
94 rendered using some function of the photodetector voltage as the contrast quantity.

95 A fundamental question presents itself naturally; what is the physical content of the
96 voltage in regards to the surface under study? Answering this question is tantamount to learning
97 which tip-sample interaction forces are at play in producing a motion of the cantilever, which
98 ultimately generates the observed voltage. To build the voltage-to-force connection, it is
99 necessary to have a reliable mathematical model that produces the kinematics of the cantilever.
100 This model is then used to answer several questions. How does the tip sensor move under
101 external forces? How does that induced motion effect a photodetector voltage? How does one
102 solve the inverse problem whereby the experimental voltage, conventionally known only from
103 the motion at one location on the cantilever, is used to reconstruct the motion of the cantilever at
104 all points and for all times, and in due course, the sought forces acting on it?

105 Usually, a minimalistic connection is made between forces and voltages where, via
106 simplifying approximations, the voltage is proportional to the force at every instant. The
107 corresponding underlying assumptions, that the cantilever's deflection at its free end is
108 proportional to the slope there, and a one-degree-of-freedom-cantilever, are too stringent for
109 quantitative force analysis when the system is far from equilibrium.[20] More accurate
110 approaches include treating the cantilever as a simple harmonic oscillator[21] and even more
111 realistically, as a true extended beam that can support spatial and temporal vibrations.[20] The
112 Euler-Bernoulli beam theory is particularly relevant to a wide range of atomic force microscopy
113 applications because the slim cantilever's vibrations are dominated by its flexural motions. In
114 effect, the Euler-Bernoulli equation provides a rigorous connection between the complete shape
115 of the cantilever and the force history required to produce that shape. Thus, if the shape of the
116 cantilever is measured experimentally and this agrees with the shape predicted by the Euler-
117 Bernoulli equation, this is synonymous with stating that the forces experienced by the system can
118 be accurately recovered using the Euler-Bernoulli equation. This is the central thesis driving the
119 work we present. The work is based on an experimental design whereby the cantilever's
120 position-vs-time curves are measured at multiple locations, not just at one point near the hanging
121 end.

122 Several previous studies have looked at the problem of validating the accuracy of the
123 Euler-Bernoulli theory in predicting the behavior of real atomic force microscope cantilevers.
124 Some of this work is reviewed below. This literature provides results that are both interesting
125 and useful to the atomic force microscopy community. However, none of the extant studies
126 simultaneously and directly compares experiment to theory for the cantilever under non-
127 equilibrium conditions.

128 Payam and Fathipour[22] performed a theoretical analysis of the Euler-Bernoulli
129 equation by means of variational analysis with the goal to incorporate practical aspects of the
130 microscope such as tip mass and cantilever geometry. Gates and Pratt[23] used Doppler
131 vibrometry in conjunction with Euler-Bernoulli analysis to measure the cantilever's spring
132 constant with high accuracy. This analysis did not address either transient behavior nor the full
133 shape of the cantilever. Payton et al.[24] tackled the problem of fast imaging whereby an
134 unknown varying force acts on the tip due to surface topography variations. While they did
135 measure the shape of the cantilever as a function of time, the study was restricted to eigenmodes
136 of the combined cantilever/sample system; amplitudes of the cantilever's vibration were
137 collected at different locations at a single frequency for times long relative to the snap-to-contact
138 event to increase reliability. This method cannot be used in our case because the snap-to-contact

139 determines naturally and suddenly what happens to the deflection of the cantilever. Zhou, Fu
140 and Li [25] used the Euler-Bernoulli theory to extract mechanical properties of composite
141 materials. While they did not deal with the full shape of the cantilever, they did compare Euler-
142 Bernoulli with finite element analysis and validated the appropriateness of Euler-Bernoulli to
143 within three percent under dynamic equilibrium conditions. Laurent, Steinberger and Bellon [26]
144 considered a cantilever with a spherical bead at its end. They compared the normal mode shapes
145 of Euler-Bernoulli theory with experimentally measured ones and got agreement to within ten
146 percent for the first four modes. While they were able to measure the shape of the cantilever at
147 multiple points versus time, they did it for normal modes and not for the general transient case.
148 Payam[27] studied the shift in frequencies due to the presence of an ambient liquid and used the
149 Euler-Bernoulli equation to analyze the signal but did not consider the shape of the cantilever or
150 transient behavior. Villanueva et al.[28] were interested in the length limits of the Euler-
151 Bernoulli equation. They found that 20 μm long levers, corresponding in their case to a
152 cantilever length:width aspect ratio of about five, are short enough to make the theory deviate
153 from experiments. Zhou, Wen and Li [29] presented a theoretical study of short cantilevers and
154 showed how to correct the Euler-Bernoulli equation via the Timoshenko theory. Their paper did
155 not present experimental comparison nor did it consider the shape of the cantilever or transient
156 behavior. Wagner and Killgore[30] studied the resonant motion of a cantilever under the effect
157 of lumped or distributed forces. No transient or experimental measurements were considered.

158 In general, the difficulty in providing a definite account of the agreement between
159 experiment and theory resides in both. On the one hand, typical atomic force microscopes are
160 not set up to measure rapid cantilever deflections at multiple points along the lever. Thus, the
161 full shape of the lever necessary to determine unambiguously the forces acting on it is not
162 available. On the other hand, the theories rely on reasonable assumptions fit to the problem of
163 interest. Thus, for example, one may be interested in cantilever free boundary conditions at the
164 hanging end for spring constant calibration, or harmonic excitations at the base for multi
165 frequency studies. All articles in this field use the Euler-Bernoulli equation with adaptations
166 pertinent to the problem at hand.

167 In this context, the present paper presents new data and analysis useful in the unsolved
168 problem of understanding the connection between theory and experiment during the snap-to-
169 contact event. We previously showed that the classic concave up surface potential vs separation
170 could be extracted from this motion in air [3] and in liquid [31]. These earlier papers utilized
171 Tikhonov regularization to solve the inverse problem imposed by only having experimental
172 measurement of the end of the lever while solution of the problem requires knowledge of the full
173 lever shape. This is an ill-posed inversion for cases involving fast transients, like in the snap-to-
174 contact. We inverted the Euler-Bernoulli equation in the cantilever's shape space spanned by the
175 normal modes under conditions of an unloaded tip. This was an intrinsically limited method
176 since, during the snap-to-contact, the tip load quickly increases thus violating the assumption of
177 an unloaded tip used to create the basis set. More recently, we developed what should be a more
178 robust method for converting the voltage-vs-time trace produced by the vertical motion of the tip
179 measured at a single cantilever location into forces, the Causal Time Domain Analysis
180 (CTDA).[32] CTDA relies on explicit consideration of the measured nonlinear voltage-time data
181 as a boundary condition to the Euler-Bernoulli equation. When we compared Tikhonov
182 regularization to CTDA, we found that the two approaches did not produce the same force-
183 separation curves.[2] An obvious next step would be to use some known surface force to
184 determine which theory performed better. However, there is currently no well-accepted standard

185 for creating a surface force that is known within a few nanometers of tip/surface contact. Thus,
186 we decided to test CTDA against experimentally measured cantilever shapes. The choice is
187 based on the fact that CTDA, unlike regularization, is free of tuning parameters. That is what we
188 present in the current article, which is organized as follows. In the Methods section, we explain
189 how conventional AFM measurements are performed and give details of our experimental setup.
190 Also, in the Methods section, a brief description of our theory is presented. Then, in the
191 Experimental Results section, we present the position versus time traces at multiple points along
192 the cantilever. In the Comparison of Theory and Experiment section, we show how the theory
193 output, i.e. the full shape of the cantilever at all times, matches with the experiment. In the last
194 section, we present the Conclusions.

195 METHODS

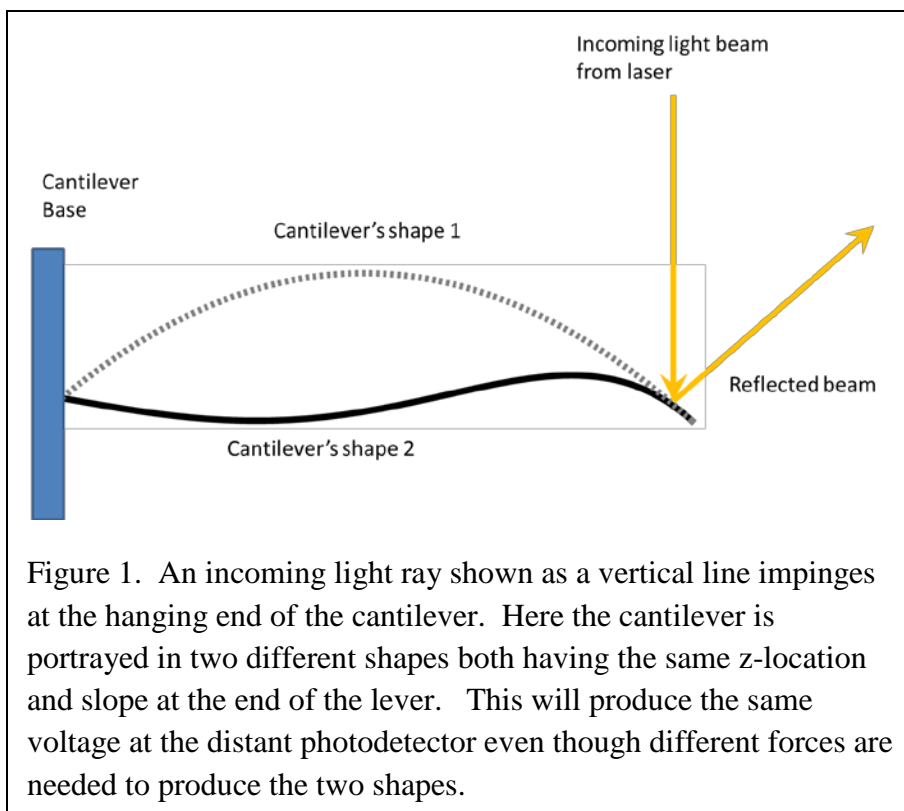
196 Conventional Experimental Approach

197
198
199
200 Standard atomic force microscopes come equipped with a light detection system to
201 measure the motion of the cantilever as shown in Figure 1. A light ray reflected off the
202 cantilever provides a photodetector voltage that is proportional to the slope of the cantilever at
203 the hanging end.

204 However, and as
205 Figure 1 depicts, the
206 instantaneous value of
207 the slope at one point
208 provides only partial
209 information of the full
210 shape of the cantilever at
211 that instant. Since the
212 full shape is necessary to
213 determine the interaction
214 force between tip and
215 sample but is not
216 typically available
217 experimentally,
218 mathematical modeling
219 is called upon to bridge
220 the gap between what is
221 needed and what
222 experiment provides.

223 One quantitative
224 approach to make the
225 connection relies on the
226 Euler-Bernoulli equation

227 to predict the motion of the cantilever.[33] In one implementation using this approach[32], the
228 instantaneous slope, proportional to the photodetector voltage, is used as a boundary condition to
229 the Euler-Bernoulli equation. By assuming a straight cantilever as an initial condition to the
230 problem, corresponding to a large tip-sample separation at the beginning of the experiment when



231 no interaction forces are detectable, the equation can be solved iteratively in time to obtain the
 232 full shape of the cantilever at all future times. With this information, the interaction force at all
 233 times is finally obtained. Afterwards, by incorporating instantaneous separation data, the sought
 234 force-separation curve is obtained parametrically in time.

235
 236 **Experimental Setup and Considerations**

237
 238 The experiment is in the form of displacement versus time measurements for many points
 239 along the long axis of the cantilever. By contrast, conventional data collection in atomic force
 240 microscopy is at a single point, typically near the hanging end of the cantilever. Laser Doppler
 241 vibrometry was used to monitor the motion of multiple points along the length of the cantilever
 242 at multiple times during the snap-to-contact. A schematic of the equipment used is shown in

243 Figure 2. The method
 244 used was similar to
 245 that described in
 246 Payton et al.[34]
 247 Briefly, a vibrometer
 248 (Polytec VIB-A-510)
 249 was attached to a
 250 cantilever mount at
 251 12.5°. This allowed
 252 for the velocity of the
 253 cantilever in the
 254 direction perpendicular
 255 to the lever's surface
 256 to be recorded with
 257 high bandwidth (up to
 258 20 MHz). The
 259 substrate (a piece of
 260 freshly cleaved mica)
 261 was cycled
 262 sinusoidally toward
 263 and away from the
 264 cantilever tip (Bruker
 265 MSNL lever B, 200
 266 μm long rectangular
 267 Si_3N_4 cantilever with a
 268 spring constant of 0.02
 269 N/m, a thermal tune

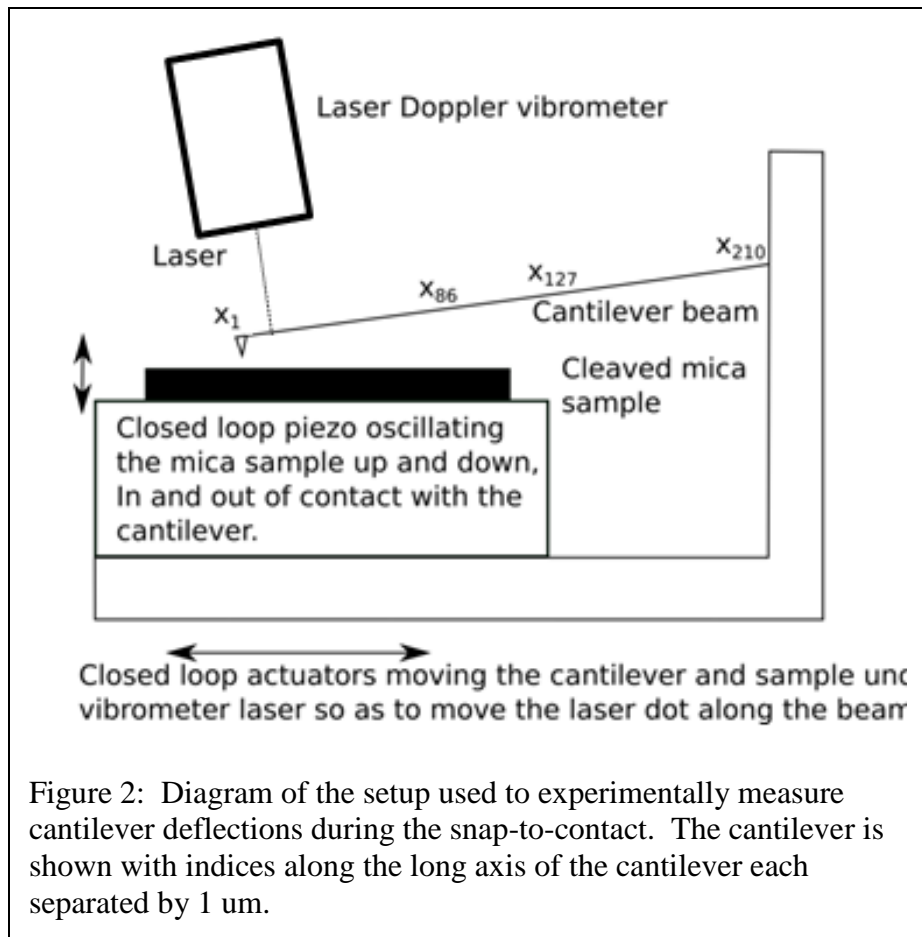


Figure 2: Diagram of the setup used to experimentally measure cantilever deflections during the snap-to-contact. The cantilever is shown with indices along the long axis of the cantilever each separated by 1 μm .

270 measured first mode resonance of 14.65 kHz, and a pyramidal tip) using a piezo stage (Npoint
 271 model NPXY60Z20) with closed loop capacitance control at 50 Hz with an amplitude of
 272 850 ± 0.1 nm (maximum velocity was therefore $267 \mu\text{m/s}$). The data displayed was collected at
 273 the point in the motion of the stage with the sample moving towards the cantilever tip at a
 274 velocity of $150 \pm 7 \mu\text{m/s}$. Z-motion monitoring was done along the cantilever every $1 \mu\text{m}$ while
 275 the cantilever underwent multiple snaps-to-contact. To do signal averaging over several snaps at
 276 the same point and to create an experimentally determined cantilever shape, it was necessary to

277 shift the individual snaps so they were in-phase with each other. This was done by cross-
278 correlating the data streams over a short time period that spanned the snap-to-contact.

279 The approach velocity was taken into account when converting the difference in piezo
280 position and cantilever deflection into tip-sample separation. Under the conditions used in our
281 manuscript, the approach velocity was very slow compared to the cantilever velocity due to the
282 snap-to-contact. So, there was unlikely to have been any significant modification in the situation
283 seen by the tip due to the moving sample. The average speed of the cantilever during the snap
284 was about 1600 $\mu\text{m/s}$. Thus, during the 25 μs of the snap as the tip traversed the 40 nm until
285 contact, the stage moved by 3.8 nm. This was taken into account when producing the force-
286 separation plots shown in the manuscript. While there was a slight drift present in the system
287 causing the tip to snap to contact with the sample at a slightly different point in the periodic
288 motion of the sample, this produced a sub-nanometer uncertainty in the tip-sample distance
289 which was within the thermal noise in the system so we chose to ignore it.

290 At much higher velocities and especially in fluid, confined fluid layer effects between the
291 cantilever and the sample surface will contribute substantially to the motion of the cantilever and
292 will need to be taken into account when determining the tip-sample force. However, none of this
293 is relevant to the problem of converting cantilever shape into cantilever force. In other words,
294 these issues are important in determining tip-sample forces, but not important in determining
295 cantilever shape.

296 Regarding non-linearity of piezo scanners, the approach was made using an Npoint stage
297 with capacitance sensor (± 0.1 nm). Any hysteresis in the motion of the piezos was taken into
298 account by using the calibrated sensor values instead of the drive signal sent to the stage.

300 **Influence of Ambient Humidity on the measurements**

301
302 The humidity was held constant at $43 \pm 5\%$ RH and a 20°C temperature throughout the
303 experiment. It is likely that the onset of the snap-to-contact was initiated due to thermally driven
304 oscillations in the fluid layers on the tip and/or mica surface. The retraction of the cantilever was
305 not the focus of the experiment therefore the formation and snapping of any meniscus was not
306 explored. It would be expected that as the humidity increased, the size and strength of any
307 meniscus force would increase, though this is not taken into account in the model used. Overall,
308 these issues are of central importance in the study of the origins of tip/sample forces probed
309 using $F(s)$ curves but not in characterizing the kinematics of the cantilever motion. For our
310 purposes, as long as some force, be it capillary, vDW, or electrostatic, was present that initiated a
311 snap-to-contact, then the lever is made to move in a non-equilibrium manner as the tip snaps
312 down to the surface.

314 **EXPERIMENTAL RESULTS**

315
316 Position vs. time traces were collected as explained in the previous section. Figure 2 labels the
317 210 positions at which time trace data were taken. We were particularly careful to gather
318 information from bending deflections only. It is known that cantilevers tend to exhibit torsion
319 upon snap-to-contact. The exact lateral location of the tip on the Bruker MSNL B cantilever
320 used is not always centered on the cantilever. Therefore, the cantilever can experience a moment
321 about the tip when the tip experiences a force such as a snap-to-contact event. The cantilever
322 displacement was measured at points taken along a line that intersected the tip. In doing so, the

323 effect of the torsional modes are minimized in the data. Data previously collected by Payton et
324 al.^{1,2} using a similar method have been shown to be modelled well by a bending mode only FEA
325 model³ indicating that, with the correct placement of the points at which data is collected, the
326 torsional modes can be ignored.

327 An example of a time trace for a single snap at a single location on the lever is shown in
328 Figure 3. To ensure that the input to our model matched the initial conditions of the theory we
329 used, it was necessary to have no displacement at early times corresponding to a motionless
330 cantilever when the tip and sample are well separated and not interacting. To achieve this, we
331 found the average displacement value prior to the snap, and then used the collected data to find
332 the last time the recorded data achieved this value prior to entering the snap-in region. We then
333 appended ten identical values of this average to the start of each snap thus guaranteeing a well-
334 behaved input.

335 At some point,
336 the tip-sample
337 interaction becomes
338 non-negligible and a
339 downward trend
340 corresponding to an
341 attraction occurs. This
342 is seen in Figure 3
343 starting at around
344 $5 \mu s$. Eventually, the
345 tip feels the repulsive
346 force due to a
347 combination of a
348 confined fluid layer
349 and Pauli exclusion
350 acting on electrons in
351 the tip and the surface.
352 This slows the
353 cantilever and
354 eventually causes it to
355 reverse direction.

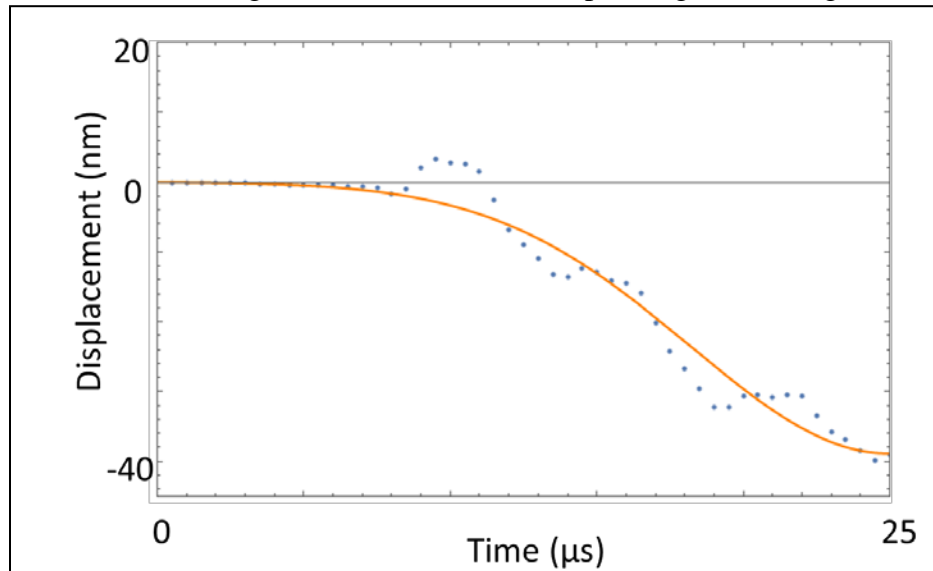


Figure 3. Snap-to-contact displacement of a point $\sim 15 \mu m$ from the free end of the cantilever as a function of time. Also shown is a best fit EVE curve[29] that helps the eye follow the general trend and is useful in matching the phases of multiple data sets like the one shown.

356 Apparent in the typical snap-to-contact event shown in Fig. 3, are a few plateaus in the
357 traverse of the cantilever toward the surface. In some cases, the path of the lever even seems to
358 reverse direction for a short time before continuing on down. It is possible that high frequency
359 oscillations of the cantilever due to the thermal bath or some other source existed as the state of
360 the lever prior to its entering the snap-to-contact regime. It is also possible that the short time
361 events came from some electronic source related to the Doppler system used to measure the
362 cantilever displacements. Conventional cantilever analysis would treat these as higher order
363 normal modes. However, the amplitude, frequency, and phase of such modes all depend
364 intimately on the boundary conditions at the hanging end of the cantilever. During snap-to-
365 contact, this boundary is changing so rapidly that the lever is unable to move through a complete
366 period of an oscillation before the boundary condition has substantially changed because the tip
367 is now closer to the surface. Thus, the concept of a mode is not well defined during the snap-to-
368 contact event. In an attempt to determine what range of frequencies the cantilever used would go

369 through as it traversed the snap-to-contact, we solved the equations 4 and 5 in reference [33]. In
 370 going from large separation to contact: the first free mode of the lever goes from 15 kHz to 0
 371 kHz, the second free mode goes from 95 kHz to 75 kHz, and the third free mode goes from 266
 372 kHz to 253 Hz. None of these ranges includes the observed oscillation frequency near 200 kHz
 373 seen in our data. This makes it unlikely that these oscillations are a reflection of higher order

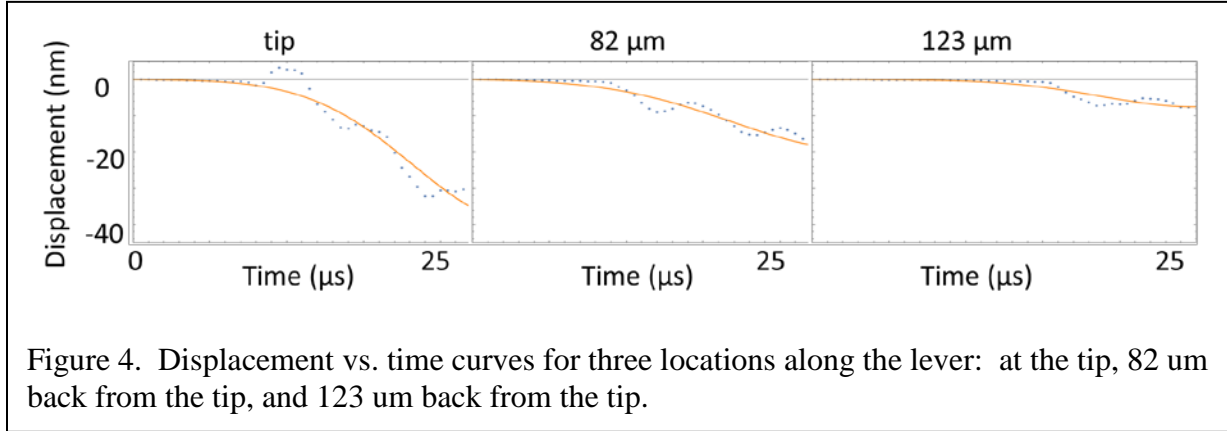


Figure 4. Displacement vs. time curves for three locations along the lever: at the tip, 82 μm back from the tip, and 123 μm back from the tip.

374 resonances in the lever. As an initial attempt at analyzing this complex data, we decided to focus
 375 on the main feature of the monotonic descent of the lever toward the surface. To extract this
 376 feature from the data, we found best-fit EVE curves[32, 35] and used these functions as inputs to
 377 our theoretical analysis.

378 Figure 4 shows three
 379 displacement vs time curves
 380 corresponding to three
 381 different locations along the
 382 cantilever. As one looks
 383 further away from the tip,
 384 the onset of the snap-in gets
 385 later in time and the
 386 amplitude of the
 387 displacement decreases.
 388 The general trend is clearly
 389 downward, however there
 390 are a few steps in the
 391 recorded path along the way
 392 as described in Figure 3
 393 above. The EVE fits are
 394 shown as the solid lines in
 395 each of the plots. In general,
 396 the EVE function fit the data
 397 very well.

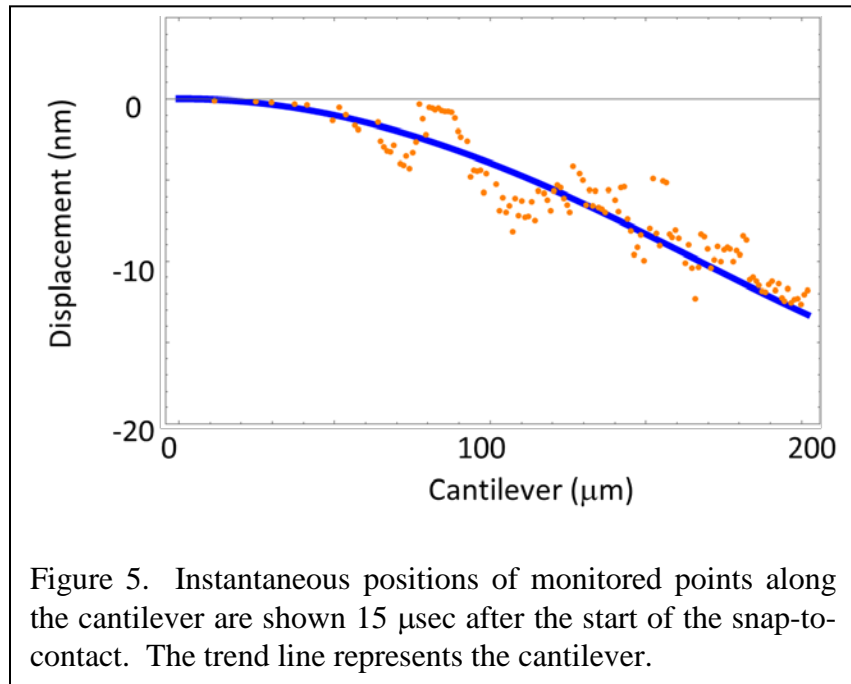


Figure 5. Instantaneous positions of monitored points along the cantilever are shown 15 μsec after the start of the snap-to-contact. The trend line represents the cantilever.

398 A useful alternative view of the cantilever motion is given in Figure 5. There, a snapshot
 399 of the full cantilever shape is created by plotting the position of each individual point along the
 400 lever at one instant in time.

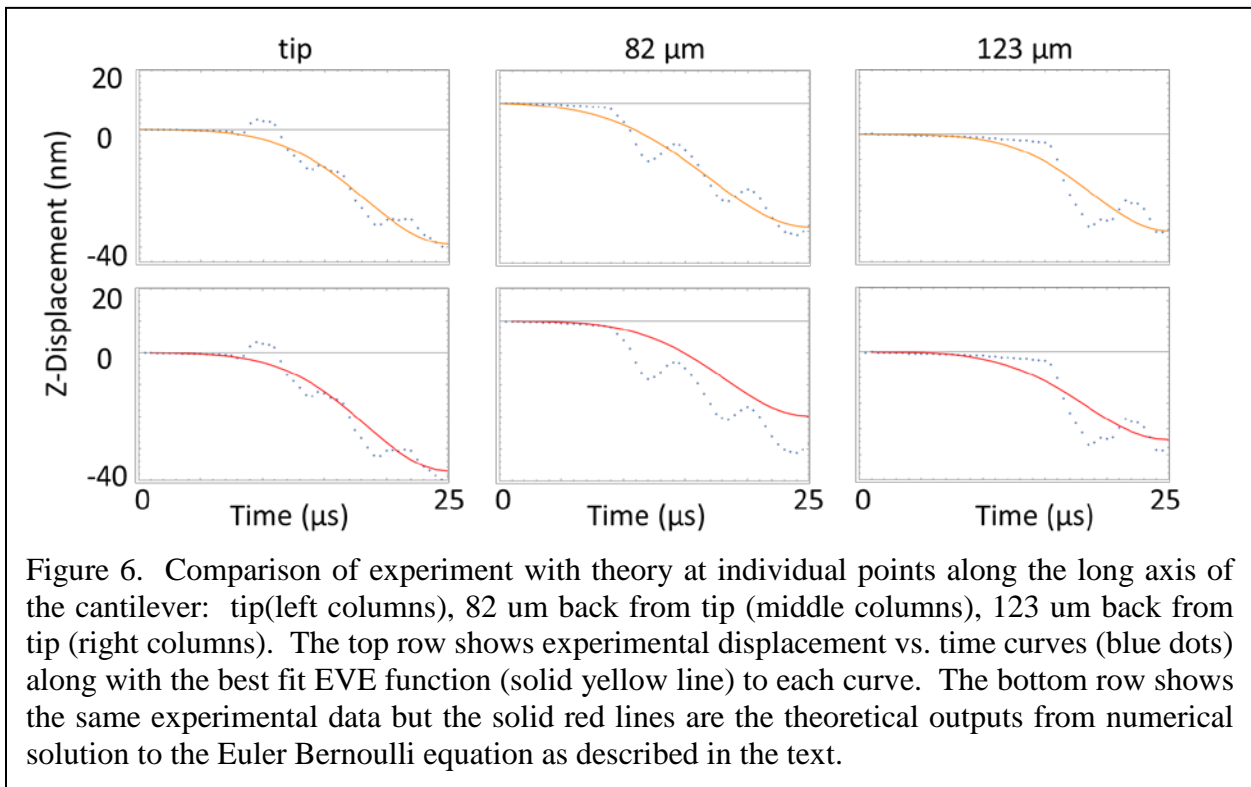
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 402

403 **COMPARISON BETWEEN THEORY AND EXPERIMENT**

404

405 Since the Euler-Bernoulli differential equation is 4th order in space and 2nd order in time,
 406 six constraints are needed to solve it. The constraints are obtained by setting two initial
 407 conditions and four boundary conditions. Our solution uses two initial conditions in the form of
 408 the shape of the cantilever at two consecutive early times. It is assumed that the force on the
 409 cantilever is small enough at these early times to allow for quasi-static motion. Thus, the two
 410 initial shapes are taken from unequivocally known static shapes under an external force at the
 411 free end. This effectively provides the initial shape of the cantilever and its initial state of
 412 velocities. In addition, we use two boundary conditions at the attached point namely, that the
 413 cantilever is fixed there and that it does not bend. The last two conditions are obtained by setting
 414 the vertical displacement and the slope at the hanging end of the cantilever equal to their
 415 experimentally measured values. With that input, we numerically solve the Euler-Bernoulli
 416 equation and predict the motion of all the cantilever points from the free to the fixed end. This
 417 theoretical cantilever shape vs time, relying only on measurements made near the free end of the
 418 cantilever, is then compared to the full experimentally measured motion along the whole
 419 cantilever.

420 To implement the solution, we took a few of the position-vs-time curves near the end of
 421 the lever and used them to determine the slope at the end of the lever. This allowed us to mimic
 422 the information available in most commercial atomic force microscopes using the direct
 423 displacement measurements provided by our Doppler technique. We emphasize that only data
 424 near the end of the lever was used to compute the entire shape of the lever. These computed
 425 shapes were then compared against the Doppler vibrometry experiments. We did this
 426 comparison in two ways. First, we looked at the displacement vs time curves for individual



427 locations along the lever. Second, we looked at the entire shape of the lever at a given time
428 point.

429 To compare theory with experiment at single points along the lever, Figure 6 shows time
430 traces at the same three points as in Figure 4 together with the theoretical outputs. The top row
431 of curves shows these experimentally determined plots with the EVE function best fits. The
432 lower set of curves shows the same experimental data but the solid lines represent the output
433 from the model which used the Euler-Bernoulli solutions using data only near the end of the
434 lever to compute the solid curves. Experiment and theory agree well at the tip (left most plots in
435 Fig. 7) which is expected since this is what was used as the input to the model. Experiment and
436 theory also fit well 123 μm back from the end of the lever. However, the fit 82 μm back from
437 the end is not as good. Looking carefully at noise in the system will allow us to determine if the
438 overall motion of the cantilever is well captured by our model or not.

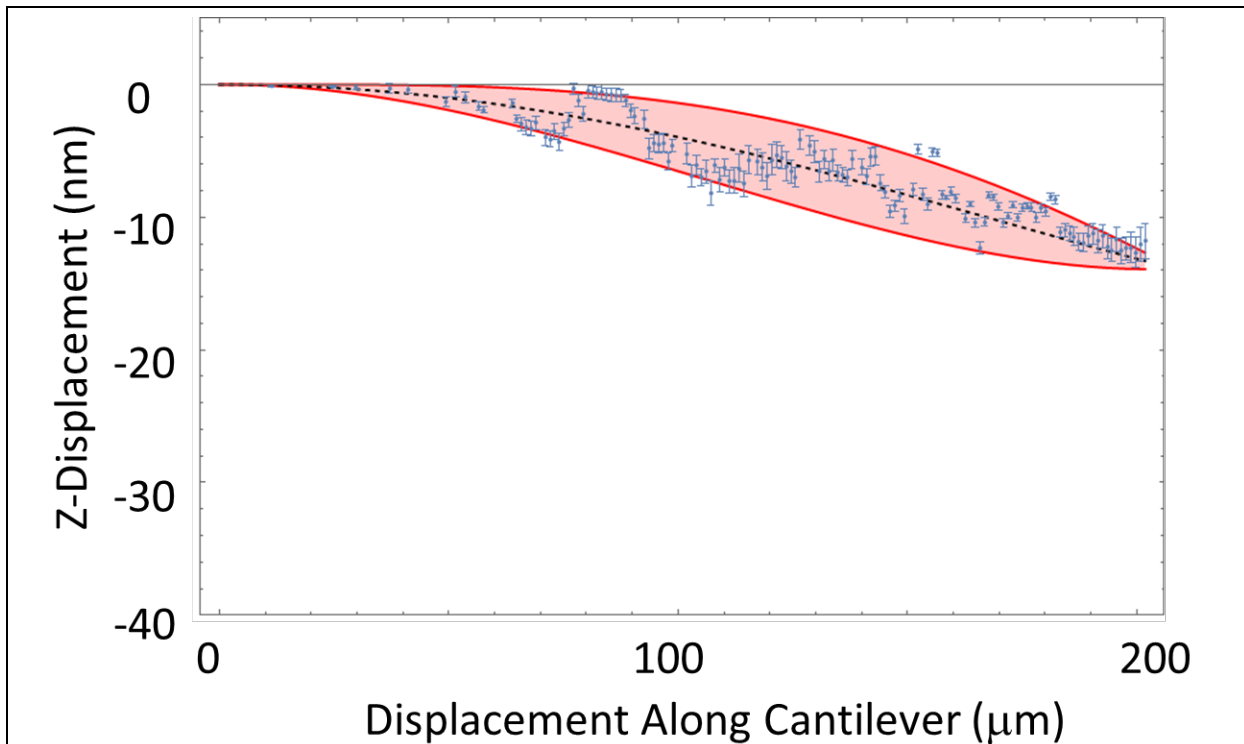


Figure 7. Snapshot of the shape of the full cantilever at an instant in time. Blue dots are the experimentally measured points. The black dotted line is the best fit to the theory. The red shaded region corresponds to the range of theoretical curves obtained using \pm one standard deviation in the experimental input error to the measured slope at the end of the cantilever.

439 Substantial measurement noise propagated from the input of our model to its output. To
440 understand how this affected the deviation between experiment and theory, it was necessary to
441 perform an error analysis that contained as much of the noise and its propagation through the
442 model as possible. To this end, we used five data points near the end of the cantilever to
443 determine its slope. In the absence of noise, any pair of these five points would have yielded the
444 same slope. Because of the presence of noise, we obtained a population of slopes from all pair
445 combinations and used this to compute a standard deviation of the noise. This population was
446 used in the analysis that follows to find an envelope of model shapes of the cantilever.

447 As a second way to compare experiment with theory, a typical snapshot of the lever with
 448 errors displayed is shown in Figure 7. The blue points with small error bars represent the
 449 experimentally determined locations of the lever at that particular location along the long axis of
 450 the lever. The dashed black line corresponds to the average theoretical value for the z -position
 451 of each location along the long axis of the lever. The shaded region represents the error in the
 452 model output based on the measured error in the input data. Specifically, five locations near the
 453 end of the lever were used. These locations were close enough together so that they should have
 454 all produced the same slope. In fact, they provided a range of slopes. The standard deviation of
 455 the slope was found and then the mean plus or minus one standard deviation was used as an input
 456 to the model. This produced a range of shapes that falls within the shaded region. Note: this
 457 slope is used as an input at each time point in the model. Thus, a different standard deviation
 458 and a different shaded region were computed at each time point.

459 Figure 8 shows six different snapshots of the snap-to-contact portion of the curve
 460 displayed in the same way as Figure 7. A movie showing the whole trajectory of the whole
 461 cantilever during the snap-to-contact corroborates what is displayed in Figure 8 (see
 462 supplemental data). While there are some experimental points that fall outside the shaded
 463 region, it is clear that the majority of experimental points fall within the computed error. For the
 464 six typical snapshots shown in Figure 9, an average of 71% of the experimental points fall within
 465 one standard deviation of the mean. Assuming a Gaussian distribution of the experimental
 466 points about some “true mean,” the obtained distribution of experimental points about the
 467 theoretical curves is as expected.

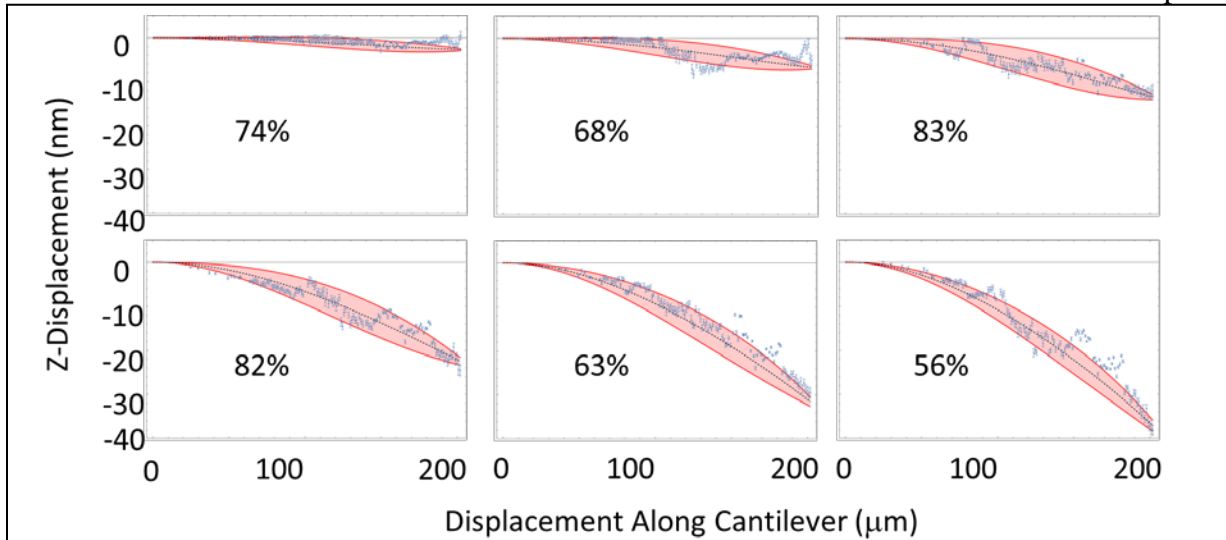


Figure 8. Superimposed experimental measurements and theoretical predictions based on the Euler-Bernoulli equation. Experimental results are shown as dots. Theory is displayed as a dashed line representing the best fit cantilever shape with a shaded region around it representing theoretical outcomes that fall within one standard deviation of the experimental means assuming normally distributed errors. Percentages reflect how many of the experimental points fall within the shaded regions around the theoretical curves.

468 This gives substantial evidence that the Euler-Bernoulli equation in general, and our
 469 model for solving the ill-posed problem present when trying to convert the data provided by
 470

471 most commercial atomic force microscopes into known cantilever shapes, provide correct
472 solutions.

473

474 **CONCLUSIONS**

475

476 We find that the Euler-Bernoulli theory is an appropriate framework to predict the kinematics of
477 the cantilever during the far-from-equilibrium snap-to-contact event. We show by direct
478 comparison with Doppler vibrometry experiments the validity of the force-separation
479 reconstruction algorithm based on the Euler-Bernoulli equation. Specifically, we did this
480 comparison for the case of a cantilever undergoing far-from-equilibrium motion driven by non-
481 linear forces during the snap-to-contact event. The relevance of our result is that, unlike in the
482 experiment used here, conventional atomic force microscopy experimental conditions allow
483 collection of the slope or position vs time at only a single point on the cantilever. While our
484 rendering of the Euler-Bernoulli-based algorithm allows for the reconstruction of the full shape
485 of the cantilever at all times, the reliability of these shapes rests ultimately on the validity of the
486 model used. Our proof thus paves the way to use our reconstruction algorithm under
487 conventional atomic force microscopy operating conditions. The time-consuming multiple
488 Doppler vibrometry measurement, while central to our test, is shown here to be no longer needed
489 when running conventional atomic force microscopy experiments. Indeed, once one knows that
490 Euler Bernoulli can be used during snap-to-contact to predict the shape of the cantilever, the
491 bending forces are readily attainable. In other words, our results should extend the ability to
492 produce accurate force-separation curves from conventional voltage-time traces into far-from-
493 equilibrium motion and non-linear interactions.

494

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496

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