Effect of undercut on the resonant behaviour of silicon nitride cantilevers

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Abstract
We present a systematic investigation of the dynamic properties of silicon nitride cantilevers in air. The thermal noise spectra of cantilevers have been measured using a home-made optical deflection setup. Torsional and flexural resonances up to the seventh mode are observed. The dependence of resonance frequencies on the dimensions and mode number is studied in detail. It is found that undercut increases the effective length of the cantilever by a value $\Delta L$, which depends on the undercut distance and the resonance mode shape, but not on the cantilever length. Finite element modelling confirms these experimental findings. A simple model is suggested for the shape of the undercut region, which agrees well with experimental findings. Using this model, the undercut cantilever can be approximated by a stepped beam, where the clamp distance depends on the underetch duration and the mode shape.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Cantilever systems in the micro- and nanometer regimes have attracted great interest because of their wide range of sensor applications. Examples, both in fundamental and industrial areas, include Casimir force detection [1], material properties analysis [2, 3], magnetic resonance force microscopy (MRFM) [4] and extremely sensitive mass sensors [5–7]. Using the first natural frequency of the cantilevers for detection [8, 9], the mass sensitivity can be in the order of $10^{-19}$ g (Hz)$^{-1/2}$ which is suitable for single virus detection. Interest in higher modes is raised as they potentially offer higher sensitivity [10, 11]. New measuring techniques are currently investigated to realize on-chip readout at resonance frequencies on the order of MHz up to the GHz range [12].

In practical applications, such as scanning probes and mass or stress sensors, often silicon nitride cantilevers are used, with dimensions in the range of ten to several hundreds of micrometers. The present work is a systematic investigation of the resonance frequency as a function of dimensions of such cantilevers in air. The undercut is explicitly taken into account [2, 3]. Flexural and torsional resonances have been measured up to the seventh mode using the thermal noise spectra. With the presented results, the resonance frequency can be predicted more accurately from the design. This is of great importance in the design of cantilever sensors (arrays) and in appropriate analysis of cantilever material properties [2]. The latter aspect is the more so important when size-dependent behaviour may enter the cantilever characteristics upon further miniaturization.

2. Fabrication

2.1. Fabrication of cantilevers with undercut

Cantilevers with undercut are fabricated from home-made Low-Pressure Chemical Vapour Deposited (LPCVD) silicon nitride [13] on silicon (1 0 0). The SiN$_x$ thickness ranges from 74 to 850 nm. The cantilever length varies from 25 to 100 $\mu$m and the width from 8 to 17 $\mu$m. For patterning of the SiN$_x$ layers a two-layer resist is used: HSQ e-beam resist (Fox-12, 200 nm) on top of the photoresist (HPR, 0.5–1.5 $\mu$m thickness, depending on the SiN$_x$ thickness). The HPR layer serves as an extra dry etch mask while etching the SiN$_x$ layer (see figure 1).
of 500 nm. The membrane is spin coated with HPR (900 nm) photoresist and on top HSQ (Fox-12, 200 nm) e-beam resist. After e-beam patterning and development the cantilevers are released using the same sequence of O$_2$ and O$_2$/CHF$_3$ plasma steps indicated for the undercut devices. The schematics of the fabrication process are shown in figures 3(a)–(b). An example of fabricated cantilevers without undercut is shown in figure 3(c).

3. Measurement setup

The resonance behaviour of the cantilevers is measured in a home-made optical laser deflection setup operating in atmospheric environment. Figure 4 depicts the configuration of the setup. The deflection of the cantilevers due to thermal noise is probed by a 658 nm (New-Focus) laser diode. The output signal, the voltage difference generated by the reflected light focused on a two-segment diode, is measured with a spectrum analyser to obtain thermal noise spectra. The laser power is typically positioned at the end of the cantilever with a spot diameter of 6 μm and a power of a few mW. The electronic bandwidth of the setup is 5 MHz and its sensitivity is estimated to be about 1 pm (Hz)$^{-1/2}$. We have reduced the laser power by a factor of 2 and found that the noise spectra are not affected. Therefore, the measured spectra are attributed to thermal fluctuations and not to excitations induced by the laser.

Thermal noise spectra are measured for a large number of cantilevers with varying length ($L$), thickness ($t$) and width ($w$). Figure 5 shows three spectra of a 74 nm thick cantilever. Flexural modes (upper panel: modes 2–6 are clearly visible in this case) and torsional modes (middle panel: modes 1–5) can be measured independently [14] by rotating the cantilever with respect to the incoming laser beam. The insets in figure 5 schematically show the movement of the reflected laser beam on the two-segmented photodiode. Flexural movements of the cantilever result in horizontal beam deflections (top figure 5), which can be detected since the laser generates a periodic signal on the two-segmented photodiode. In this configuration, the detector is insensitive to the vertical beam deflections which represent the torsional movements. In the middle figure 5 the sample has been rotated by 90°. Now
torsional movements can be detected and for the flexural modes the output voltage equals zero. When the sample is placed at 45°, the reflections from the flexural and torsional modes make an oblique movement and both modes are detected at the same time. The independent identification of the modes is an advantage of measuring thermal noise spectra; measurements on actuated cantilevers generally show the two types of modes at the same time [15].

The resonance frequency and the $Q$-factor of the resonances are determined from Lorentzian fits (red lines) through the data, as is illustrated in figure 6 for the fourth torsional and flexural modes. In the next sections, we will discuss in more detail the dependence of the resonant frequencies on the cantilever geometry.

4. Flexural modes

The equation of motion for the flexural vibration modes in vacuum (quality factor $Q \gg 1$) and its solutions can be found in the text books [16, 17] and is briefly summarized here for convenience. We will adopt the notation shown in figure 7 and note that the starting point for the calculation of the resonance frequencies is the Euler–Bernoulli beam equation:

$$EI \frac{d^4y}{dx^4} + \rho A \frac{d^2y}{dt^2} = 0,$$

(1)

where $E$ is the Young's modulus, $I$ is the area moment of inertia, $\rho$ is the mass density, and $A$ is the cross-sectional area.

The harmonic vibration solution can be found using the method of separation of variables with $Y(x, t) = u(x) e^{i\omega t}$, which simplifies (1) for the spatial solution to

$$\frac{d^4u(x)}{dx^4} - k^4u(x) = 0,$$

(2)

where

$$k^4 = \frac{\rho A(2\pi f)^2}{EI}$$

(3)
the dependence of the fundamental resonance frequency is in agreement with (6). The dependence of $f_n/f_1$ and $f_n/f_1$ in good agreement. The error in all measurements of $f_n$ was within ±10 Hz.

For cantilevers, the boundary conditions are

$$u(0) = \frac{du(0)}{dx} = \frac{d^2u(L)}{dx^2} = \frac{d^3u(L)}{dx^3} = 0.$$  

A non-trivial solution for the prefactors in (4), leads to the characteristic equation

$$1 + \cos(k_n L) \cos(k_p L) = 0.$$  

The solutions $\{\alpha_n = k_n L\}$ of (5) give the wave numbers $k_n$ of a set of flexural vibration modes, where $n$ is the mode number. Combining the solutions of (5) with (3), one finds the resonance frequency of the cantilevers in terms of the dimensions and the material properties:

$$f_n = \frac{\alpha_n^2}{2\pi \sqrt{12}} \frac{t}{L^2} \sqrt{\frac{E}{\rho}},$$  

where we have substituted $A = wt$ and $I = wt^3/12$.  

For the first seven modes the mode-dependent $\alpha_n$ is given by 1.8751, 4.694, 7.855, 10.996, 14.137, 17.278 and 20.420, respectively. With these numbers the ratio $f_n/f_1$ is calculated as shown in table 1. Equation (6) is to within a 2% error valid for rectangular cantilever plates (thin beams) with a small aspect ratio ($L/w > 1.5$) [18]. Experimental values determined from a 200 nm thick cantilever are given in the same table; they are in good agreement with the theoretical values. For other cantilevers we also find $f_n/f_1$ values that are close to those listed in table 1. We note that a slightly better agreement can be obtained if we correct the frequencies for the low $Q$-factors. In the harmonic approximation, the correction equals $1 - (1/(4Q^2))^{1/2}$ [19] and the ratios are then equal to 6.34, 17.81, 36.18, 57.29, 84.42 and 117.59, respectively.

To further test the applicability of the Euler–Bernoulli theory, we have measured the resonance frequencies as a function of length, thickness and width. Figure 8 shows the dependence of the fundamental resonance frequency $f_1$ versus $L^{-2}$ in samples without undercut. The observed linear dependence is in agreement with (6). The dependence of $f_1$ on the thickness is shown in figure 9, for cantilevers with a fixed undercut. For a fixed cantilever length, a linear behaviour is observed, in accordance with (6).

### Table 1. The frequencies and $Q$-factors of the first seven flexural modes of a cantilever with dimensions ($w \times L \times t = 17 \times 100 \times 0.2 \, \mu m^3$). The theoretical and experimental $f_n/f_1$ are in good agreement.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$f_n$ (MHz)</th>
<th>$Q$-factor</th>
<th>$f_n/f_1$ (theory)</th>
<th>$f_n/f_1$ (exp)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.032</td>
<td>2.2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0.21</td>
<td>13.3</td>
<td>6.267</td>
<td>6.51</td>
</tr>
<tr>
<td>3</td>
<td>0.59</td>
<td>35.2</td>
<td>17.548</td>
<td>18.29</td>
</tr>
<tr>
<td>4</td>
<td>1.26</td>
<td>66.2</td>
<td>34.389</td>
<td>35.87</td>
</tr>
<tr>
<td>5</td>
<td>1.90</td>
<td>92.8</td>
<td>56.843</td>
<td>59.15</td>
</tr>
<tr>
<td>6</td>
<td>2.80</td>
<td>124</td>
<td>84.914</td>
<td>87.93</td>
</tr>
<tr>
<td>7</td>
<td>3.90</td>
<td>~100</td>
<td>118.599</td>
<td>121.54</td>
</tr>
</tbody>
</table>

5. **Torsional modes**

Apart from the flexural modes (the $xy$-plane) the cantilever also has other degrees of freedom. Vibration in the $xz$-plane is also possible although in practice the amplitudes of those modes are much smaller and more difficult to detect due to a higher stiffness ($I = tw^3/12$ instead of $I = wt^3/12$). Torsional modes refer to displacements due to rotation around the cantilever $x$-axis and the corresponding resonance frequencies of these modes are within our detection range. The equation of motion is given by [20]

$$T \frac{\partial^2 \theta}{\partial x^2} - \rho I_p \frac{\partial^2 \theta}{\partial t^2} = 0,$$

where $T$ is the torsional stiffness, $\theta(x, t)$ is the angle of twist about the $x$-axis (figure 7), and $I_p$ is the polar moment of inertia given by

$$I_p = I_x + I_z = \frac{wt^3}{12} + \frac{tw^3}{12}.$$
for the cross section in the yz-plane. In practice, $t^3 w \ll tw^3$ so that the first term can be neglected.

The torsional stiffness $[21] T = \eta G$ in which the shear modulus $G$ is given by $G = E/(2(1 + \nu))$, with $\nu$ being Poisson’s ratio. The factor $\eta$ is dependent on the geometry of the cross section and will be discussed later. By the method of separation of variables $[22]$

$$\frac{d^2 \Theta(x)}{dx^2} + \lambda_n^2 \Theta(x) = 0, \quad \text{with} \quad \lambda_n^2 = \frac{\rho I_p}{T} \omega^2. \tag{7}$$

The general solution to (7) is

$$\Theta(x) = b_1 \sin(\lambda_n x) + b_2 \cos(\lambda_n x),$$

with boundary conditions:

$$\Theta|_{x=0} = T \frac{\partial \Theta}{\partial x} \bigg|_{x=L} = 0.$$

The latter term indicates that there is no torque applied at the free end of the cantilever and from this boundary condition one obtains the characteristic equation:

$$\cos(\lambda_n L) = 0, \quad \text{with} \quad \lambda_n = \frac{(2n-1)\pi}{2L}$$

so that

$$f_n = \frac{2n - 1}{4L} \sqrt{\frac{\eta G}{\rho I_p}}. \tag{8}$$

The remaining problem is to find the value of $\eta$. When the cross section of the beam is considered to be an ellipse with the axis lengths equal to the width $w$ and the thickness $t$ of the cantilever, then $\eta = t^3w/3$ and the resonance frequency in the absence of damping equals

$$f_n = \frac{2n - 1}{2L} \sqrt{\frac{G}{\rho t w}}. \tag{8}$$

For a narrow rectangular shaped beam, a better approximation is given by $[23]$

$$\eta \approx \frac{1}{3} w t^3 \left(1 - 0.630 \frac{t}{w}\right).$$

For the beams in this study, the difference between these two approximations is less than 1% and we will use (8) to calculate the resonance frequencies for the torsional modes.

Figure 10 shows the resonance frequencies of the first torsional mode for a sample without undercut. The frequency versus reciprocal length does not show the expected linear dependence (8). An upward curvature is observed instead: shorter cantilevers have a higher resonance frequency than that expected from (8). This can be explained by taking into account the ratio $L/w$ of the cantilever, according to the theory of Reissner and Stein $[24]$. With the measured Young’s modulus obtained from the flexural modes (200 GPa for the cantilevers released by wet etching), and the Poisson’s ratio of 0.22 from literature $[25]$, we have calculated the torsional resonance frequencies predicted by this theory. As figure 10 shows, the data are in good agreement with this calculation.

6. The effects of undercut

6.1. Flexural modes

To investigate the effect of undercut on the cantilever resonance frequency, we now turn to the length dependence of modes in the samples with undercut. The inset of figure 11 shows the result. The undercut, which is 12.5 $\mu$m in this sample, leads to a deviation from the linear relation predicted by (6) and observed for devices without undercut in figure 8. The deviation from linearity is most pronounced for short cantilevers. Apparently, the base region near the anchoring point participates in the overall resonance behaviour of the cantilever. The effect of undercut can be included by adding a length $\Delta L$ to the nominal cantilever length $[26–28]$, where $\Delta L$ is independent of the length of the cantilever. Thus
the ‘effective length’ of the underetched cantilever is given by \( L + \Delta L \). By performing a least-square fit (fit function: \( f(x) = a/(L + \Delta L)^2 \)) through the resonance frequency data with \( \Delta L \) and \( a \) as free parameters, \( \Delta L \) was determined to be 6.7 \( \mu m \) for the data shown in figure 11. With the inclusion of \( \Delta L \), a linear relation between the resonance frequency \( f_1 \) and \( 1/(L + \Delta L)^2 \) is obtained, as illustrated in figure 11.

A similar analysis has been performed on three other batches of samples with undercuts of 10.4 \( \mu m \), 15.4 \( \mu m \) and 20.7 \( \mu m \). The linear relation between \( f_1 \) and \( 1/(L + \Delta L)^2 \) is restored for \( \Delta L \) equal to 2.8, 8.4 and 11.2 \( \mu m \), respectively. These fit values are plotted versus the experimental undercut distance \( L_u \), as shown in figure 12 for the first resonance frequency (circles). The undercut distance, \( L_u \), has been determined from SEM inspection.

For higher mode numbers, we also found a discrepancy between \( f_0 \) and \( L^{-2} \). Again, an effective length can be defined to restore the expected linear behaviour between the two parameters. The dependence of \( \Delta L \) on the first three flexural modes has been investigated for 200 nm thick cantilevers and we find an increase of \( \Delta L \) as the mode number increases: \( \Delta L = 5.3 \mu m \) for \( n = 1 \) (slightly smaller than the value for the 500 nm thick cantilevers; see figure 12), \( \Delta L = 7.8 \mu m \) for \( n = 2 \) and \( \Delta L = 8.6 \mu m \) for \( n = 3 \). Apparently, for the higher modes an increasing part of the base participates in the vibration.

To support the experimental findings a three-dimensional finite element simulation was carried out in ANSYS using 20 node structural solid elements (SOLID186 and SOLID95) and an element size of 1–5 \( \mu m \). The undercut cantilever is modelled as a stepped beam as depicted in figure 13(a), and with a more realistic clamp which mimics the actual situation of an isotropic etching process when releasing the cantilevers (figure 13(b)). Released areas of cantilever and base regions are allowed to move freely. All translational and rotational degrees of freedom are set to zero throughout the cross section of the clamping regions where release is zero. As for input parameters the experimental value for the Young’s modulus has been used (239 GPa) whereas the density (3100 kg m\(^{-3}\)) and Poisson’s ratio (0.22) are taken from the literature [25]. The simulations show that indeed a \( \Delta L \) can be defined and its values have been determined in the same way as in the experiments, i.e., by considering the frequency versus \( L^{-2} \) dependence. Note that the results shown are from simulations with \( w_u > 10 \mu m \), where \( 2w_u \) is the total width of the simulated structure (see figure 13). In this limit, the calculated \( \Delta L \) is independent of \( w_u \). If \( w_u \) is smaller, the effective cantilever length increases since the structure becomes less stiff.

For the idealized undercut case (figure 13(a)), the grey line in figure 12 shows the experimental undercut frequency versus calculated undercut length \( L_u \). As expected, the line crosses the origin: any undercut makes the effective cantilever length larger than the defined length. This behaviour is in contrast with the experimental data points which indicate a dependence with an intercept on the x-axis around 10 \( \mu m \).

The black line in figure 12 shows the calculated \( \Delta L \) versus undercut for the fundamental mode \( f_1 \). When the protrusion is explicitly taken into account. To model the protrusion, an isotropic etching process is taken at a constant etch rate \( k \). The apex of the protruding tip, marked A, is positioned a distance \( L_u^* \) from the cantilever base (see figure 13(b)). The minimum undercut required to release the cantilever is half the cantilever width \( w \). From the geometry, the position of the support is calculated as \( L_u^* = \sqrt{(k\tau)^2 - (w/2)^2} \), where \( \tau \) is the etching time. The etch rate of the apex is found by differentiating its position to the etch time:

\[
\frac{dL_u^*}{d\tau} = \frac{k^2\tau}{\sqrt{(k\tau)^2 - (w/2)^2}} > k, \quad \text{with } k\tau > w/2. \tag{9}
\]

The apex remains sharp, as is observed in the experiment. Note that just after the cantilever is released, when \( k\tau \approx w/2 \), the apex etch rate \( \frac{dL_u^*}{d\tau} \) is high. In practice, this results in poor control over the undercut of the released cantilever right after release.

The model with protrusion (black line in figure 12) shows a much better agreement with the experimental data. For
low \( L_u \), however, the model predicts slightly higher \( \Delta L \) values compared to the measured ones. This discrepancy is attributed to a more complicated etch profile than that assumed in our 2D model. As can be seen in the inset of figure 2, the sharp underetch shape is slightly curving back towards the cantilever which makes the cantilever’s effective length shorter than modelled. For large \( L_u \), this effect becomes less pronounced, and the simulated and experimental values coincide. We also modelled the higher modes. As in the experiment, we find a slight increase of the \( \Delta L \) values with increasing mode number.

Figure 14 shows a comparison between the calculated resonance frequencies of the first bending mode versus underetch for the two models. As expected, the effect of the protruding support vanishes when the underetch length \( L_u > w \). For underetch lengths up to the cantilever width, the protrusion plays a significant role. For small undercuts \( (L_u < 0.5 \, w) \) the cantilever length effectively becomes much shorter than \( L \) as only the outer tip of the cantilever is released. We note that for the description of the undercut on flexural modes, a reasonable approximation can be obtained by assuming a straight clamp at \( L_u^* \), as shown by the dotted line in figure 14. Here, \( L_u^* \) can be calculated using (9). The underetch region is then simplified to a stepped beam geometry, which has been studied in the past [29].

6.2. Torsional modes

For torsional resonances the effect of the protrusion is expected to be less pronounced, as the support concentrates at the cantilever central length axis, which is a nodal line. The inset of figure 14 shows the dependence of the resonance frequency on \( L_u \), simulated using the models in figures 13(a) and (b). In contrast to the bending modes, for the torsional modes the role of the protrusion is indeed insignificant: the base can be simplified as if it were clamped at \( L_u \). This means that the stepped beam model of figure 13(a) can be applied. Note that it does not mean that the effective cantilever length increases by this amount, as we will show below.

Figure 15 shows the measured fundamental torsional resonance frequency versus the reciprocal length for 200 nm thick cantilevers with an undercut of 10 \( \mu \text{m} \). Simulations (grey line) agree well with the experiments. The torsional frequencies according to Reissner and Stein theory, which takes into account the aspect ratio \( L/w \) [22], but not the undercut, are also plotted (black line). In this particular case, the effect of undercut is compensated by the decreasing \( L/w \) aspect ratio, and as a result (8) gives a good approximation to the data (dashed line).

As with the flexural modes, in the case of torsional modes the effective cantilever length is larger than the physical length. For the data in figure 15, we estimate a \( \Delta L \) of 3.7 \( \mu \text{m} \), which is different from the corresponding value of the flexural modes.

7. Summary and conclusions

We have studied the resonance behaviour of silicon nitride cantilevers in air, and compared the experimentally obtained results to existing beam and plate theories, and finite element simulations. Torsional and flexural modes can be distinguished in the thermal noise spectra by rotating the sample over 90°. For both types of vibrations, higher modes are observed. The flexural modes of cantilevers without undercut behave according to the Euler–Bernoulli theory. However, the presence of undercut results in a significant deviation from this theory. We show that a correction can be made to the nominal cantilever length to restore the relation between frequency and length. This correction is independent of the cantilever length, but varies with mode number. In the case of the torsional modes also a deviation due to the undercut has been observed, but different from the flexural mode observations. Finite-element simulations of the resonance frequency behaviour of the various modes are in good agreement with the experiments and support our findings.
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