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Improved V-shaped microcantilever width profile for sensing applications

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Abstract
In this work we have proposed an improvement in the shape of the V-shaped microcantilever by varying the width profile. In this paper we have studied the variation of resonant frequency as a function of changes in profile determined by the length of the microcantilever, keeping constant the active area for binding. It is observed that for the optimized nonlinear profile the angle at the tip is 91.41°, more than twice the angle at the tip of the linear profile cantilever. The variation of the equivalent spring constant with changes in the profile is also studied. It is proposed that the optimum nonlinear profile cantilever has a spring constant of $\sim 0.39\,\mu\text{N}\,\mu\text{m}^{-1}$. The resonant frequency is obtained by using the Rayleigh–Ritz method, the deflection model and the SUGAR simulator. The results are compared and an improvement in the performance of the cantilever is observed.

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

1. Introduction

Microcantilevers are some of the earliest and most elementary MEMS devices and have been used in many applications. Atomic force microscopy (AFM) and various applications that have enabled nanotechnology rely mainly on microcantilevers. Over the last few years, these cantilever systems have provided a new platform for sensing chemical and biological materials and for a better understanding of their reaction mechanisms. The performance of microcantilevers is determined by various parameters such as stiffness, quality factor and resonant frequency. With the goal of improving the performance, various researchers have studied and developed models for understanding cantilever behaviour [1–5]. There is always a trade-off between parameters such as deflection and the resonant frequency [6]. In AFM, cantilevers sense forces and when the deflection of the cantilever is measured optically, good deflection capability is required. For biological applications, surface effects play an important role and the binding can be related to changes in the resonant frequency. High sensitivity is prevalent in systems with higher resonant frequency [1]. The active region available on the upper surface of the cantilever is also an important parameter for chemical or biological sensors. Different cantilever parameters are weighted according to the requirements of the application for optimizing the performance. Rectangular, V-shaped and T-shaped cantilevers are the most commonly used cantilever geometry for sensors. V-shaped cantilevers, with reduced lateral twisting due to their geometry, have so far been analysed using the parallel beam approximation (PBA) [7]. The V-shaped cantilever, with linear arms, has been equated as the difference of two solid triangles and the resonant frequency has been obtained using energy balancing principles and the Rayleigh–Ritz (RR) method [7].

To date, many new models have been developed for improved microcantilever profile for sensing applications [6–8], but no work has been reported earlier that discusses the variation in the width profile of a V-shaped microcantilever.

In this work, we optimize and improve the V-profile to get an improved resonant frequency using the variation in the width profile of a microcantilever and propose an analytical model of the equivalent spring constant of the structure assuming that the deflection is small and hence suitable for linearization. The mass distribution of the cantilever also decides the resonant frequency. Since different parts of the cantilever vibrate with different amplitudes, the direct mass of the cantilever does not provide a clear correlation between the resonant frequency and the physical dimensions. In this work the total sensing area on

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the cantilever surface has been maintained constant and the thickness is not varied.

2. Theory

When a system is forced into oscillations, the frequency of the driving force decides the amplitude and a peak response is obtained at the resonant frequency. The fundamental resonant frequency decides the mass sensitivity of cantilevers and assuming that the added mass causes negligible variation in the stiffness of the cantilever, the change in the resonant frequency of cantilevers is obtained as [1]

$$\frac{\Delta f}{\Delta m} = -\frac{1}{2}\frac{f_0}{m}, \tag{1}$$

where Δf is the change in the resonant frequency, Δm is the mass binding on the cantilever surface, f_0 is the fundamental resonant frequency and m is the cantilever mass. For a greater change in frequency, i.e. better mass sensitivity, the required value of f_0 is very large. Modelling this frequency is an important step towards the total analysis of cantilevers.

2.1. Existing model

Considering a linear V-shaped cantilever with E as the Young's modulus, ρ as the density, H as the cantilever thickness, $W(x)$ as the varying width and l_1 as the length, from the symmetry of the V-shaped cantilever and by using the RR method the resonant frequency and $W(x)$ are given as [7],

$$f(W(x)) = \frac{H}{2\pi}\sqrt{\frac{3E}{\rho}}\sqrt{\frac{\int_0^L W(x)(l_1-x)^2\,\mathrm{d}x}{\int_0^L W(x)x^4(3l_1-x)^2\,\mathrm{d}x}}, \tag{2a}$$

$$W(x) = \begin{cases} \dfrac{W_1}{2}\left(1-\dfrac{x}{l_1}\right) - \dfrac{W_0}{2}\left(1-\dfrac{x}{l_0}\right) & x \in [0, l_0], \\ \dfrac{W_1}{2}\left(1-\dfrac{x}{l_1}\right) & x \in [l_0, l_1], \end{cases} \tag{2b}$$

where W_1 is the width of the outer triangle, W_0 is the width of the inner triangle and x is the distance along the direction shown in figure 1. The V-shaped cantilever is assessed as the difference of a smaller triangle from the outer triangle. L_1 is the length of the outer triangle and L_0 is the length of the inner triangle. Assuming $\rho = 10^4\,\mathrm{kg\,m^{-3}}$, $E = 10^{10}\,\mathrm{Pa}$, $H = 1\,\mu\mathrm{m}$ and keeping the dimensions of the outer triangle as $L_1 = 100\,\mu\mathrm{m}$ and $W_1 = 80\,\mu\mathrm{m}$, using (2a) and (2b), the variation of the resonant f with the dimensions of the inner triangle, i.e. in the inner gap, is shown in figure 2. The maximum resonant frequency of ~33 KHz is obtained for a V-structure with no gap in the centre, i.e. a simple solid triangular cantilever beam [7].

2.2. New model: second order profile microcantilever

In the existing works, the width profile of the V-shape has been considered to be linear. In this section, we investigate the effects of choosing a general second order profile and

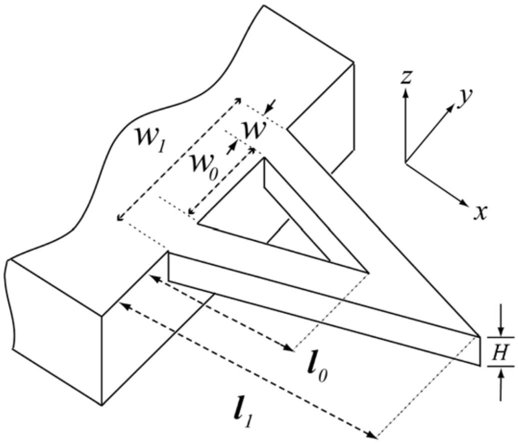

Figure 1. Structure of a general V-shaped microcantilever.

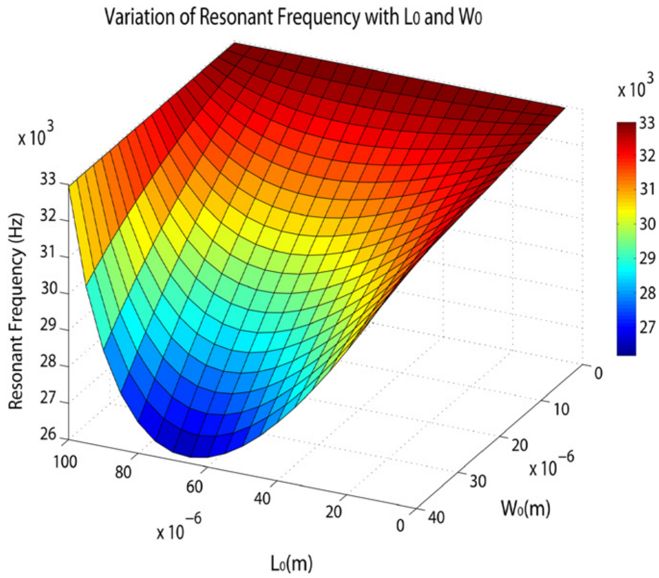

Figure 2. Variation of the resonant frequency f with change in dimensions L_0 and W_0 of the inner cantilever gap.

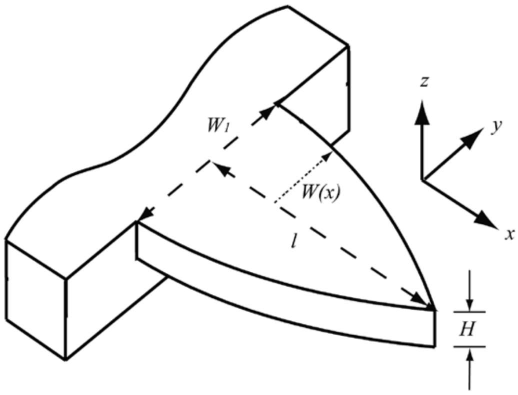

Figure 3. Structure of a proposed V-shaped microcantilever with a nonlinear width profile.

then proceed to optimize the coefficients. Using the result of the previous model, a microcantilever with no internal gap is considered. Symmetry is maintained about the x-axis. Figure 3 shows the microcantilever with a nonlinear width

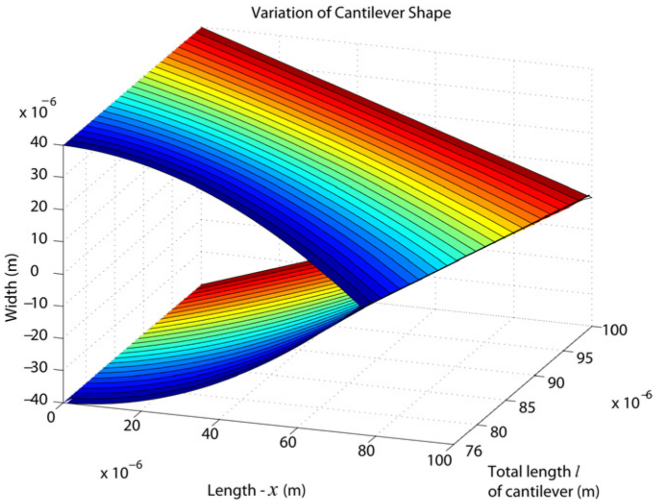

Figure 4. Variation of the cantilever boundary with change in l. The shape corresponding to $l = 100\,\mu$m is the triangular cantilever.

profile. The profile on one half of the microcantilever is given by a general second order polynomial,

$$W(x) = ax^2 + bx + c \tag{3}$$

with the following conditions, existing in the linear profile, to retain the salient features of the V-shape:

$$W(0) = \frac{W_1}{2}, \qquad W(l) = 0, \qquad W'(x) \leqslant 0, \qquad x \in [0, l], \tag{4}$$

where l is the length of the nonlinear profile microcantilever and $W(x)$ is the half width of the microcantilever as a function of x. Conditions in (4) also ensure that the maximum width in any resulting profile is W_1 and is retained at the fixed end. The area on top of the proposed nonlinear profile microcantilever, $A_{\rm nl}$, is the active sensing area and is kept the same as the area of the triangular microcantilever, A_l, obtained in the existing model. This can be expressed mathematically as

$$A_{\rm nl} = 2\int_0^l W(x)\cdot {\rm d}x = A_l = \frac{1}{2}W_1 l_1. \tag{5}$$

Using (3), (4) and (5), the coefficients can be determined as a function of one independent variable l, and the final expression for the profile is given by

$$W(x) = \left(\frac{3W_1 l - 6A_l}{2l^2}\right)x^2 + \left(\frac{3A_l - 2W_1 l}{l^2}\right)x + \frac{W_1}{2}. \tag{6}$$

The value of l independently decides the profile and is a parameter that decides the resonant frequency. Figure 4 shows the cantilever shape as a function of the total length using the same dimensions and material constants as those mentioned in the previous subsection. A vertical cross section along the length–width plane in figure 4 represents the top view of the cantilever profile. The minimum limit for the total length l is decided by (4) and (5). The starting value of l is $\sim 76\,\mu$m. Here, the lower limit is set by the condition $W'(x) \leqslant 0$. There is no mathematical constraint on the maximum value of l.

2.3. Effective spring constant

Let the deflection of the cantilever be $v(x)$ along the length of the cantilever. The second order differential equation of the bending function is given by [7]

$$\frac{{\rm d}^2 v(x)}{{\rm d}x^2} = \frac{F}{EI}(l - x), \tag{7}$$

where F is the applied force, E is Young's modulus, I is the cross-sectional area moment of inertia. The area moment of inertia varies as

$$I(x) = \frac{2W(x)H^3}{12}. \tag{8}$$

Since $W(x = l) = 0$, $W(x)$ is modified as

$$W(x) = ax^2 + bx + c = a(x - l)(x - p), \qquad p = \frac{c}{la}, \tag{9}$$

where l and p are the roots of $W(x)$.

Hence equation (7) becomes

$$\frac{{\rm d}^2 v(x)}{{\rm d}x^2} = \frac{-6F}{aEH^3(x - p)}. \tag{10}$$

Integrating (10) twice, and using the boundary conditions, $v(x = 0) = 0$ and $v'(x = 0) = 0$, the deflection function $v(x)$ is obtained as

$$v(x) = \frac{6F}{aEH^3}[(x - p)(1 - \ln(x - p)) + \ln(-p)x + p(1 - \ln(-p))]. \tag{11}$$

For small deflections the effective spring constant $K_{\rm eff}$ is given by

$$K_{\rm eff} = \frac{F}{v(l)} = \left\{\frac{6}{aEH^3}[(l - p)(1 - \ln(l - p)) + \ln(-p)l + p(1 - \ln(-p))]\right\}^{-1}. \tag{12}$$

To study the influence of the mass on the resonant frequency, the calculation of the effective mass is essential. Effective mass will also provide an alternative method to compute the resonant frequency since the equivalent stiffness is already known.

The total kinetic energy of elements of the vibrating cantilever are equated to the kinetic energy of a system with its mass equivalent to the effective mass and amplitude equal to the deflection at the cantilever tip. The energy equation is given by

$$E_{\rm cant} = \frac{1}{2}\int_0^l v(x)^2\omega^2{\rm d}m = E_{\rm mass} = \frac{1}{2}m_{\rm eff}v(l)^2\omega^2. \tag{13}$$

The value of $m_{\rm eff}$ is calculated from (13) and it is normalized with respect to the actual mass to make it a dimensionless quantity called the effective mass coefficient, $N_{\rm EM}$, which is defined as

$$N_{\rm EM} = \frac{m_{\rm eff}}{\rho A_{\rm nl} H}, \tag{14}$$

where $A_{\rm nl}$ is the top surface area of the cantilever and H is the cantilever thickness. $N_{\rm EM}$ is a fraction that decides exactly the effect of the mass on dynamic properties. Therefore the

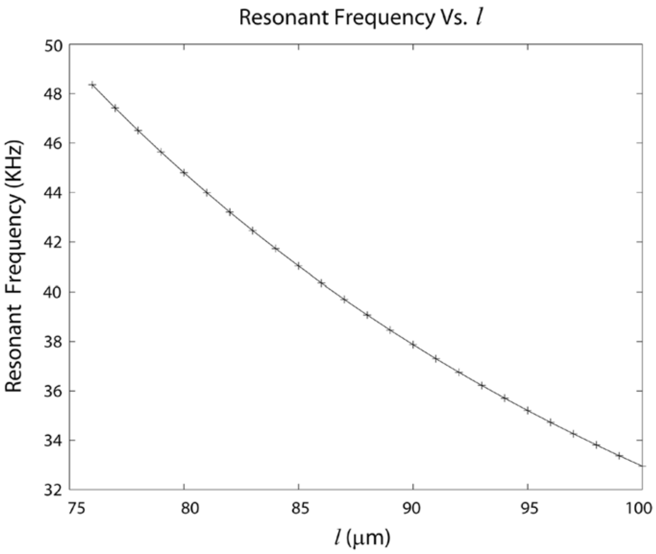

Figure 5. Resonant frequency curve for varying profiles decided by the total length of the nonlinear cantilever.

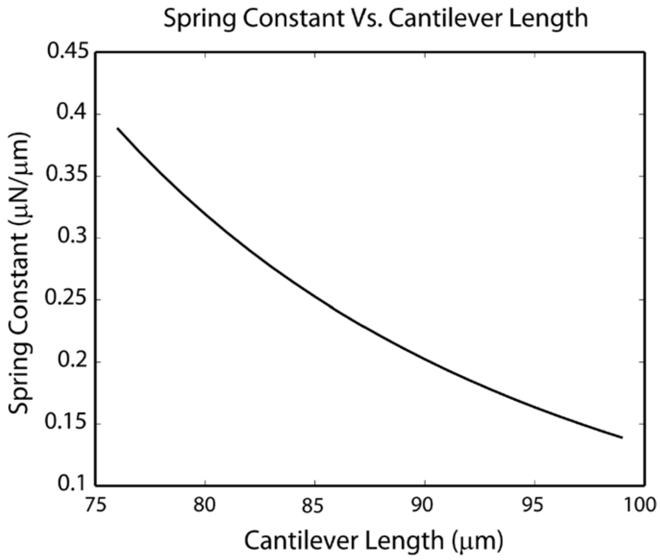

Figure 6. Effective spring constant of the structure as a function of the cantilever length.

resonant frequency of the system can be calculated by using the following relation:

$$f_0 = \frac{1}{2\pi}\sqrt{\frac{K_{\mathrm{eff}}}{m_{\mathrm{eff}}}}. \tag{15}$$

3. Results and discussion

Using (1) to (6), the resonant frequency is calculated as a function of l. In figure 5, the resonant frequency is plotted as a function of the changes in profile decided by the parameter l, keeping the active area for binding a constant. From (6), it is seen that for $l = 100\,\mu$m the coefficient $a = 0$ in (3) and the cantilever has a triangular profile as shown in figure 4, which results in a resonant frequency of 32.95 KHz seen in figure 5. The resonant frequency corresponding to the optimal value of $l = 76\,\mu$m is $f = 48.36$ KHz, an improvement of 46.77%. The trend in figure 5 indicates that a decrease in the length of the cantilever leads to an increase in the resonant frequency. However, it is not advantageous to make extremely small cantilevers as it reduces the area available for sensing and the deflection reduces very markedly. Higher resonant frequency restricts the amplitude of the effects of external noise and short cantilevers also show more resistance to thermal noise making our proposed model more insensitive to noise.

In [6], variation in the thickness profile has been proposed as a method to improve the cantilever performance parameters. Despite the improvements, it is practically very difficult to produce cantilevers with continuously varying thickness profiles such as triangular or quadratic profiles. In our proposed model, the profile variation suggested is only for the width and is decided by the design of the mask used in the photolithography step of the fabrication process.

The variation of the equivalent spring constant with changes in the profile is shown in figure 6. It is seen that the stiffness reduces as the length of the cantilever increases.

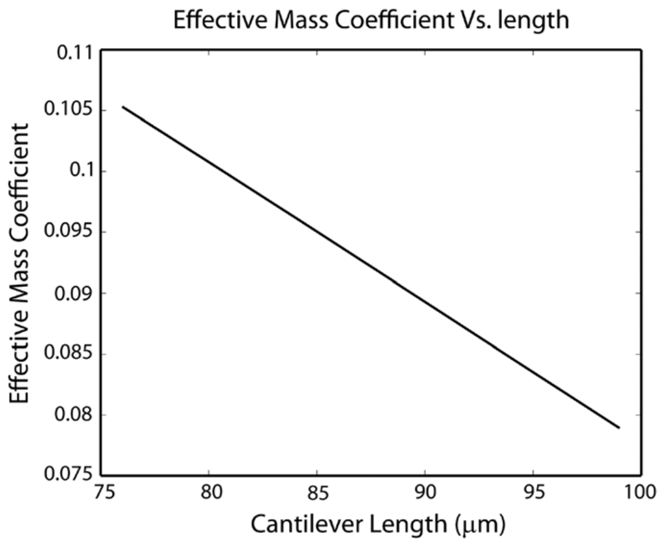

Figure 7. Effective mass coefficient of the structure as a function of the cantilever length.

The proposed optimum nonlinear profiles cantilever has a spring constant of $\sim 0.39\,\mu\mathrm{N}\,\mu\mathrm{m}^{-1}$. The variation of the effective mass coefficient is shown as a function of the length of the cantilever in figure 7. It is seen that the effective mass coefficient decreases almost linearly with the increase in the length. This is used to further calculate the resonant frequency of the improved V-shaped microcantilever as a function of its length.

Figure 8 shows the variation between the angle subtended at the tip of the V-shaped microcantilever as a function of its length. It is observed that the angle subtended at the tip of the linear V-shaped cantilever is 43.6°. As we know, sharp corners are very prone to overetching during the process of fabrication. After photolithography and development, the patterned layer with openings is used to differentially etch the underlying layer where the actual cantilever will be formed. At this stage, the presence of sharp corners leads to excessive undercutting.

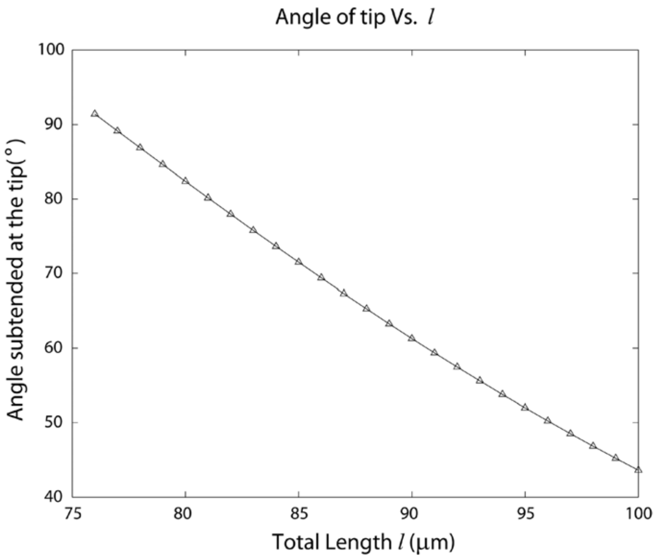

Figure 8. Variation of the angle subtended at the tip of the V-shaped microcantilever as a function of its length.

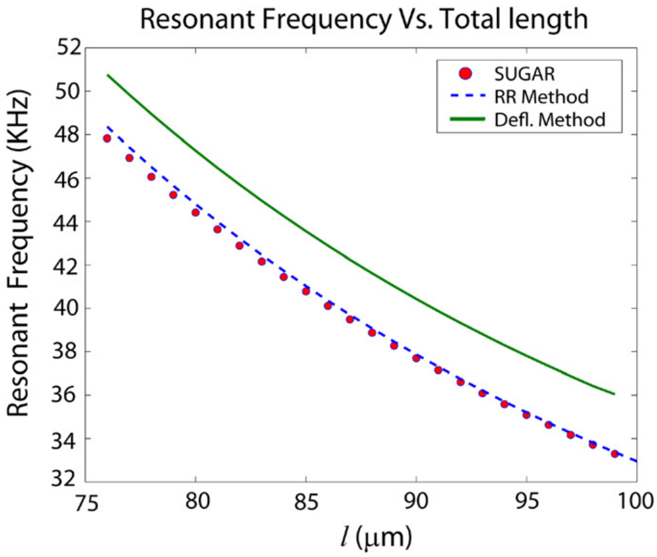

Figure 9. Comparison of the resonant frequency of the V-shaped microcantilever as a function of its length obtained from different methods.

Convex corners are sites of preferential etching, undercutting and get rounded very easily [9]. Convex corner compensation is essential for structures with very sharp features. For V-shaped microcantilevers, the final length is very sensitive to overetching because of the sharp corner at the free end of the cantilever. In many applications of cantilevers such as in AFMs, the structure of the cantilever tip is extremely important. From figure 8 it is observed that for the optimized nonlinear profile, the angle subtended by the tangents at the tip is 91.41°, more than twice the angle at the tip of the linear profile cantilever. Compared with the linear cantilever the proposed profile has larger resistance to convex corner undercutting resulting from the larger angle tip.

The resonant frequency has been modelled using two different approaches. In order to verify these results, the simulation of the proposed nonlinear cantilever is done for varying profiles using the SUGAR simulator. The nonlinear width profile of the cantilever was obtained by merging 100 rectangular beams of different widths. Figure 9 shows a comparison of the resonant frequency values obtained from the RR method, the deflection model in (15) and using the SUGAR simulations. The result of the RR method is shown by a dashed curve, values obtained from (15) are plotted as a continuous curve and the SUGAR simulation results are indicated by circular points. It is observed that the three results show a common trend. The governing equations of the finite element method and the RR method are similar and the results obtained from the SUGAR simulations and the RR method also show close resemblance. The effective mass and effective spring constants obtained for the calculation of resonant frequency using the deflection method are obtained after assuming linear behaviour and small displacements. The assumption of linear spring stiffness and the use of numerical methods for calculating the effective mass may be responsible for the slight deviation of the resonant frequency values obtained using the deflection method shown in figure 9, but this method is important as it also involves two other parameters, effective mass and stiffness, that provide a qualitative understanding on the influence of the cantilever profile on the resonance frequency. The calculation of the effective mass coefficient will also be applicable while considering the response to mass addition over the complete top surface. The results of the three methods shown in figure 9 confirm the improvement in the resonant frequency with reducing length and increasing nonlinearity.

4. Conclusion

We have proposed an optimized nonlinear width profile with improved performance parameters. Keeping the maximum sensing area and width at the fixed end constant, the proposed profile has greater resonant frequency and reduction in convex corner undercutting compared with the linear V-shaped profile. The final length of the cantilever is less sensitive to process variations such as overetching and undercutting because of the intrinsic large angle tip of the proposed profile. Thus the variation in the width profile provides a new potential method for improving the performance of microcantilevers.

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