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Optimal Design and Evaluation of Cantilever Probe for Multifrequency Atomic Force Microscopy

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1. Abstract
In multifrequency atomic force microscopy (AFM) to simultaneously measure topography and material properties of specimens, it is highly desirable that the higher order resonance frequencies of the cantilever probe are assigned to be integer harmonics of the excitation frequency. In this paper, a structural optimization technique is employed to design cantilever probes so that the ratios between one or more higher order resonance frequencies and the fundamental natural frequency are ensured to be equal to specified integers. A one-layer probe with variable width is optimally designed for assigning single and multiple resonance frequencies. Moreover, a three-layer model is proposed to provide more frequency choices. All the designs are verified by experiments, through the focused ion beam (FIB) milling based fabrication technique and AFM measurement.
2. Keywords: Multifrequency atomic force microscopy, Cantilever probe, Eigenfrequency, Structural optimization, Focused ion beam

3. Introduction
Among various atomic force microscopy (AFM) techniques, tapping mode is particularly attractive for imaging soft specimens because it does not suffer from lateral friction, hence having minimal damages to a soft specimen as well as to probe tip. In the tapping mode, a probe is excited at or near its fundamental resonance frequency, and its tip touches the sample surfaces once in every oscillation. A feedback controller is used to keep the vibration amplitude at a constant level by adjusting the height of probe base or sample table, to provide the topography of the specimen.

Conventional tapping mode AFM involves the excitation and detection at a single frequency component of the tip's motion, inevitably losing the information contained in other harmonic components. In recent years, tapping mode AFM is emerging to excite or/and detect at multiple frequencies to maximize the potential of AFM for characterization, defined as multi-frequency AFM [1].

Periodic tapping between the probe tip and the sample surface produces a periodic pulse-like tip-sample interaction force, and it was observed that the response of probe due to such a tip-sample force contains rich information about material properties of the sample, which can be observed in the higher harmonics of the response [2]. In practice, however, there exists a significant difficulty. Because the responses at higher harmonics are typically several orders smaller in magnitude than that at the excitation frequency, and also because applying a large tapping force is not suitable for high resolution imaging, a reasonable signal-to-noise ratio at the higher harmonics is not readily available [3].

According to the theory of vibration, if the frequency of a higher harmonic is equal to one of the resonance frequencies of the probe, the response of the probe at such a frequency can be greatly enhanced. However, in regards to the commonly used rectangular cantilever probe, their high order resonance frequencies do not naturally align with any one of the harmonics [1]. Therefore, the probe should be redesigned [4]. Sahin *et al.* [5] designed a cantilever probe with a notch whose third order flexural resonance frequency was equal to the 16^{th} harmonic and the probe is called a harmonic cantilever. But this design has a limited capability and a general methodology is not available. Li *et al.* [6] attached a concentrated mass to the probe to tailor the second and the third order eigenfrequencies to be integer multiplies of the fundamental eigenfrequency. If large change of the frequencies is required, the mass needs to be heavy. As a consequence, this will lower the fundamental resonance frequency of the probe. Xia *et al.* [7] employed the level set based topological optimization method to design harmonic probe. But the result is not practical from manufacturing and structure stability issues, and also only one order eigenfrequency assignment is achieved.

For imaging material composition, several harmonics are required to accurately reconstruct the tip-sample interaction force, and they should lie in the frequency range with high sensitivity, typically in a low range for soft materials and a high range for hard samples. Therefore, a practical methodology is needed to design harmonic probes with pre-determined eigenfrequencies. Actually, this type of structural optimization problem with eigenfrequency requirement has been a subject of extensive interests and investigations in past decade. Maeda and Nishiwaki [8] designed the vibrating structures that targets desired eigenfrequencies and eigenmodes shapes. Meske *et al.* [9] introduced a new optimality criteria method to handle eigenfrequency problems. And Du and Olhoff [10] applied SIMP method and bound formulation to maximize eigenfrequencies and frequency gaps. Tsai and Cheng [11] utilized SIMP method and MAC to obtain desired eigenfrequencies and mode shape.

Here, this study proposes a design framework for developing a practical novel probe to meet the demands of multifrequency AFM. There are two types of design to demonstrate. The first design is one-layer design with variable beam width. Another design is three-layer design with symmetric top and bottom layers, whose width are the design variables, while the middle layer is kept constant.

4. Optimization design

With above defined cantilever design specification, the task now is to devise an optimal design to ensure that the set of M orders $I = \{I_1, I_2, \cdots, I_M\}$ of cantilever resonance frequencies match the required set of M harmonics $J = \{J_1, J_2, \cdots, J_M\}$ according to

$$\omega_{I_k} = \Omega_{J_k} = J_k \omega_1, \qquad k = 1,2,\cdots,M \tag{1}$$

Optimization technique is employed here as a systematic approach. The design variable for one layer design is the cross-sectional width along the beam length. However, only the width of symmetric top and bottom layer is chosen as the design variable for three-layer design.

The major optimization goal is to satisfy the resonance harmonics assignment constraints. For nano-scale imaging, the effective spring constant K_1 of the fundamental mode is also required to be high. Also higher excitation frequency brings higher scanning rate. Therefore, the objective is to maximize the fundamental resonance frequency, setting the function $\lambda_1 = \omega_1^2$. Thus the design optimization problem is described as follows with multiple frequency constraints:

$$\begin{aligned} &\text{Max } \lambda_1 = \omega_1^2 \\ &\text{Such that: } \lambda_{I_k} - J_k^2 \lambda_1 = 0, \quad k = 1,2,\ldots,M \end{aligned} \tag{2}$$

The weak form of the state equation for eigenvalue problem is given by

$$a(u,v) = \lambda b(u,v), \forall v \in U \tag{3}$$

where $a(u,v) = \int_\Omega C_{ijkl} u_{kl} v_{ij} dV$ and $b(u,v) = \int_\Omega \rho u_i v_i dV$. Here, the displacement field *u* defines the mode shape of the eigenvalue problem in bilinear form for structure domain Ω. *U* denotes all kinematically admissible displacement fields and *v* is the test function. *C* and ρ denote the elasticity tensor and material density respectively.

In the present study, analysis of AFM cantilever probe with variable width and constant thickness distribution is modeled by the Bernoulli-Euler beam theory. The slenderness ratio of bending in vertical direction for most commercial probes is larger enough to justify the use of Bernoulli-Euler beam theory [12]. During practical tapping mode AFM detection process, the optical detection of the probe mainly involves the vertical bending mode. Vibration in other directions is neglected. For instance, torsional signal is filtered out at signal analysis step for this kind of measurement.

5. Evaluation

We started the design with a commercial probe stock (AppNano, FORTA). Nominal specifications of the silicon probe include: length 225 µm, width 27 µm, thickness 2.7 µm, spring constant 1.6 N/m, and fundamental frequency 61 kHz. Real dimensions of the probe were also measured, and they were used in the optimization. The material properties of silicon is 2330 kg/m^3 in density and 169 GPa for the Young's modulus of bending in <110> direction since the probe is made from standard (100) silicon wafer. In addition, mass of the probe tip was considered in the computation, and it was evaluated from scanning electronic microscopy (SEM) images, which approximately accounts for 3% of total mass. The picket-shape end of the probe remained unchanged in the design.

5.1 One-layer design

The first case of optimization was to achieve $\omega_2/\omega_1 = 6$, i.e., matching the second resonance frequency to the 6th

harmonic. Based on the optimized design shown in Fig. 1(a), the cantilever is fabricated from a commercial rectangular probe by modification of its width-profile using focused ion beam (FIB) milling (FEI Quanta 200 3D FIB). The ion beam energy and current were 30 kV and 5 nA, respectively. Fig. 1 (b) shows the SEM image of the probe obtained. The as-prepared probe was then installed on an AFM (Bruker Bioscope) to measure its resonance frequencies. In Fig. 1 (c), the first two resonance peaks f_1 (64.24 kHz) and f_2 (387.26 kHz) are shown. The ratio between f_2 and f_1 is 6.03, which is fairly close to our design expectation.

Another case of optimization was to simultaneously achieve two integer frequency ratios $\omega_2/\omega_1=6$ and $\omega_3/\omega_1=17$. Fig. 2 (a) shows the design result. After FIB milling, the as-prepared probe, shown in Fig. 2 (b), was measured for its resonance frequencies, which are shown in Fig. 2 (c). Here, we only concern with the peaks of flexural vibration. The first three resonance frequencies are 61.96 kHz, 369.35 kHz and 1056.3 kHz, respectively. The ratio values of f_2/f_1 and f_3/f_1 are 5.96 and 17.05, respectively.

It is worthy to note that the fabrication of the final probe was achieved through several rounds of local modifications, in consideration of the differences of the cross-section shape between the computational model and the real probe. The cross section of the real probe stock is not truly rectangular, but it is treated as rectangular in the computational model for convenience.

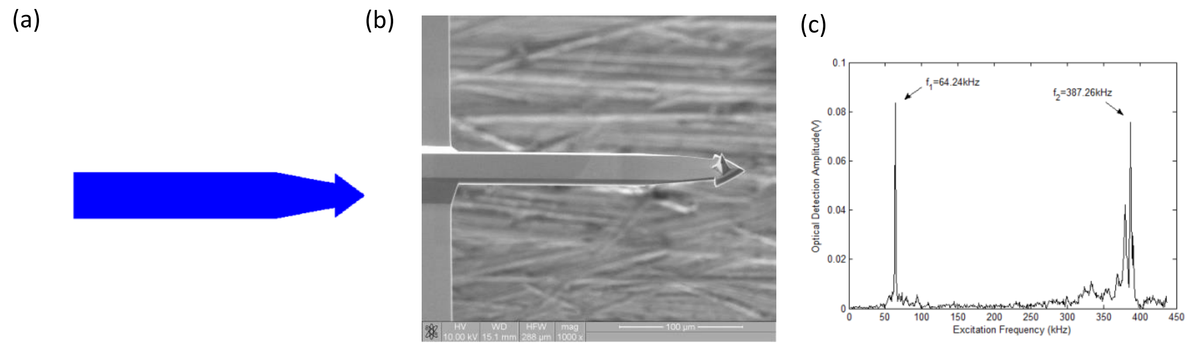

Figure.1 (a) Optimally designed result with frequency constraint $\omega_2/\omega_1=6$; (b) SEM image of probe after FIB milling; (c) Frequency spectrum of fabricated probe

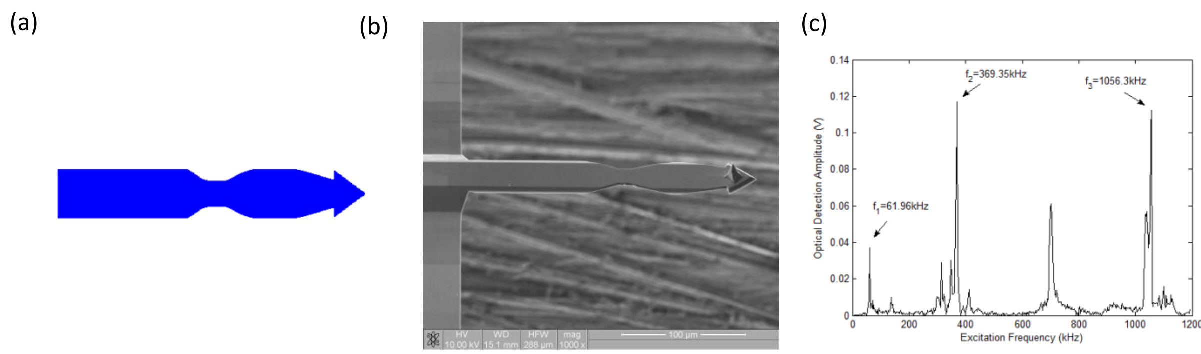

Figure.2 (a) Optimally designed result with frequency constraints $\omega_2/\omega_1=6$ and $\omega_3/\omega_1=17$; (b) SEM image of probe after FIB milling; (c) Frequency spectrum of fabricated probe

5.2 Three layer design

Three-layer design provides larger capability for tailoring frequencies. The design domain of three-layer design is broader than that of one-layer design, since the width of top and bottom layer can be zero, which is avoided in one-layer design. The real dimension of probe thickness is 2.8 µm. And we set the thickness of top and bottom layer as 0.7 µm. Thus the maintained middle layer has a thickness of 1.4 µm.

The first case of optimization is to achieve $\omega_2/\omega_1 = 4$. Fig. 3 (a) shows the pattern of top and bottom layer. Based on this design, we fabricate the probe using FIB milling. The ion beam energy and current were 30 kV and 3 nA, respectively. Fig. 3 (b) and (c) demonstrated the probe from front and back view, respectively. Fabricated probe is then installed on AFM to measure its resonance frequencies. In Fig. 3 (d), the frequency peaks are 78.89 kHz and 320. 79 kHz, which means that the ratio between f_2 and f_1 is 4.07.

The second case of optimization is to simultaneously achieve $\omega_2/\omega_1=6$ and $\omega_3/\omega_1=14$. Fig. 4 (a) shows the pattern of top and bottom layer. Fig. 4 (b) and (c) present the front and back view of the FIB milled probe, respectively. Fig. 4 (d) demonstrates the frequency spectrum obtained from AFM measurement. The first three flexural resonance frequencies are 77.34 kHz, 455.94 kHz and 1093.6 kHz, respectively. The ratio values of f_2/f_1 and f_3/f_1 are 5.90 and 14.14, respectively.

Precise depth control of FIB milling is difficult, such that the final milled depth of top and bottom layer are achieved by several rounds. Also, the final pattern is obtained after several local modifications.

6. Conclusion

In summary, a systematic structural optimization method is presented to design harmonic cantilever probes. The ratios between one or more higher order resonance frequencies and the fundamental natural frequency are made to be equal to specified integers, while the fundamental natural frequency is maximized. The approach is demonstrated with one-layer and three-layer designs. Examples of tailoring single and multiple frequencies are presented. The harmonic probes designed through the optimization approach were fabricated using the FIB technique. Their resonance frequencies were measured, and the results verified the effectiveness of the probes of our design.

7. Acknowledgements

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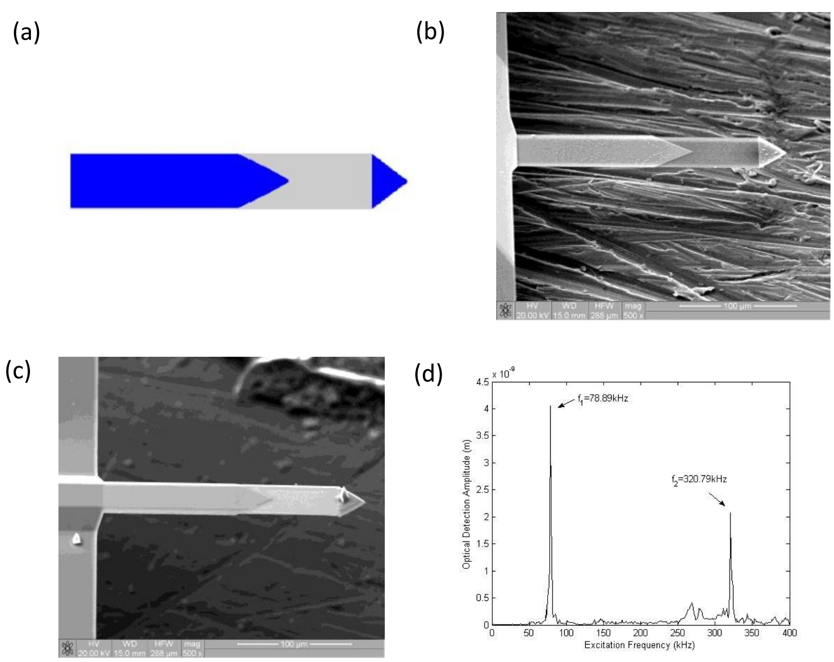

Figure. 3 (a) Optimally designed top and bottom layer pattern with frequency constraint $\omega_2/\omega_1=4$; (b) SEM image of probe's front side; (c) SEM image of probe's back side; (d) Frequency spectrum of fabricated probe

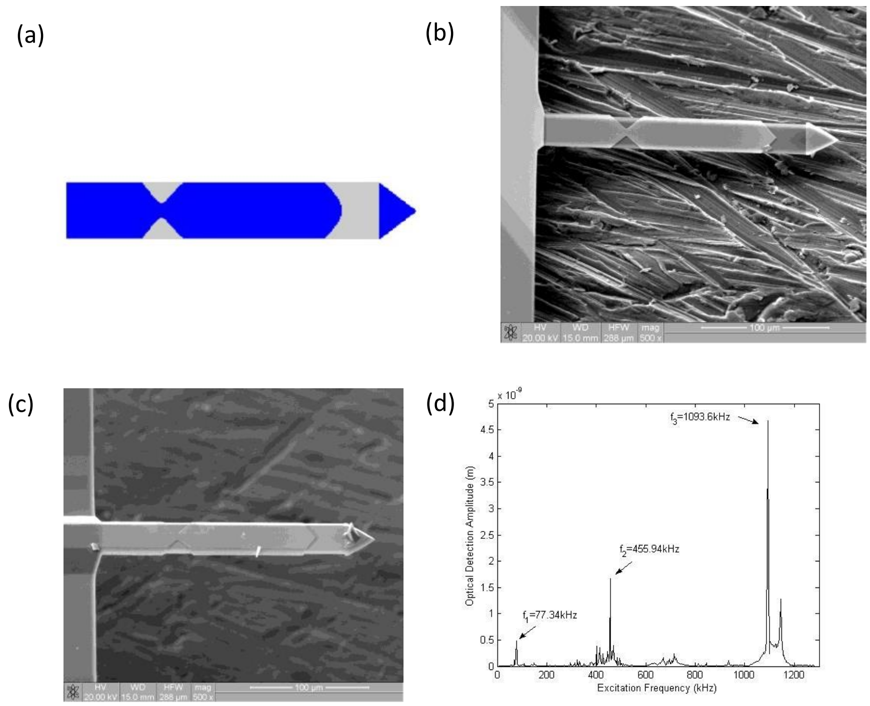

Figure. 4 (a) Optimally designed top and bottom layer pattern with frequency constraints $\omega_2/\omega_1=6$ and $\omega_3/\omega_1=14$; (b) SEM image of probe's front side; (c) SEM image of probe's back side; (d) Frequency spectrum of fabricated probe

8. References

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