Numerical Modeling of Surface Roughness Effects on the Natural Frequency of a Silicon Cantilever

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Abstract - This paper presents a numerical model showing the effects of surface roughness on the resonant frequency of a cantilever beam. The model developed incorporates non-uniform cross-sections to represent surface roughness. Results show that as roughness increases, resonant frequency increases. The model presented here also has good agreement with FEM simulations.

Keywords: Deep reactive ion etching, Finite Element Method, Microelectromechanical Systems, Surface roughness

1. Introduction

Most MEMS devices use a silicon substrate because of its good mechanical properties. Silicon is also most commonly used in MEMS to form cantilever beams. During fabrication, certain processes cause surface irregularities that influence not only the surface properties of a device but also its reliability and performance [1,4,8,9]. For cantilevers that are used for energy harvesting, this may lead to harvesting inefficiency as its operating frequency is highly dependent on its geometric shape. Etching of silicon using deep reactive ion etching (DRIE) at large etch depths results in rougher surfaces [2] due to an increased response in process pressure, amount of coil power and increased helium backside cooling readings. Note that the resulting surface roughness changes the moment of inertia per cross-section of the cantilever. This paper presents a numerical model that can be used to calculate the natural frequency of a silicon cantilever beam, which includes the effects of the cantilever's non-uniform cross-sectional heights caused by surface roughness.

2. Numerical Modeling of Surface Roughness

In approximating the natural frequency of a fixed-free cantilever beam that is subjected to free vibrations, available mathematical models assume that the cross section of the beam is uniform [5-7]. Hence, the beam's moment of inertia is considered uniform all throughout its entire length. In this paper, the numerical model incorporates both the device properties and surface roughness to predict the resonant frequency of a cantilever. To do this, measurement and characterization of the surface roughness of sample structures were performed first. These samples have undergone a standard DRIE MEMS fabrication process with an etch rate of 750 nm/cycle using C_4F_8 , SF_6 , and O_2 gases.

The root mean square roughness parameter, S_q was used for characterizing the surface roughness [3], and is obtained by squaring each height value and taking the square root of the mean. Four samples were measured at the same location per region of a 6-inch wafer and statistical information was acquired using a high-resolution 3D laser microscope. Roughness was characterized and analyzed using the microscope's software data analysis tool. Areal method was used to acquire roughness of the surface which region of measurement was specified to be 640 x 640 μ m. Sample images of the surface roughness data are shown in figure 1.

Etch depth of the wafer was measured to fairly quantify surface roughness. Thickness measurement results for a DRIE 6-inch wafer is shown in figure 2. It is found that the center region is thicker compared to other regions of the wafer. The average thickness of the center region is approximately 120 μ m while the rest of the wafer's thickness ranges from 90-100 μ m. Acquired roughness using parameter, S_q shows that the center region of the wafer tends to have an average of

approximately 2.5 µm while the left and right regions have more variations compared to the bottom, top and the center regions. Results of the measurement after characterization is shown in figure 3.



Fig. 1: Selected samples of roughness height images (1024x1024 px, 20x mag) using high resolution 3D laser microscope at 100µm thickness of a silicon wafer after 600 cycles of DRIE.



Fig. 2: Thickness variation across a 6-inch silicon wafer after performing DRIE. The center region of the wafer has the highest thickness value indicating least silicon etching rate at this region.



Fig. 3: Variation in surface roughness, S_q , across a 6inch silicon wafer after performing DRIE. It can be seen that roughness, S_q , can range from 1-4.7µm across the wafer.

Euler-Bernoulli's natural frequency equation of a cantilever beam shown in equation 1 calculates moment of inertia with the assumption that the beam's cross-section is uniform throughout its entire length. Illustrated in figure 4, is the rectangular cross-section's second moment of area on either axis with respect to its centroid given by a general form in equation 2.

$$\omega_n = \frac{1}{2\pi} \left(\frac{\beta_n}{L}\right)^2 \sqrt{\frac{E I}{\rho A}}$$
(1)

$$I = \int dI = \int_0^M r^2 dm \tag{2}$$

The differential element dm of the moment of inertia dI is defined with respect to a specific rotational axis. In figure 4a, the beam is bending about the z-axis with respect to its central axis. Figure 4b, calculates Iz across the length b and width h from the centroid and integrates all the mass elements of the cross-section. This results in a second moment of area as described in equation 2. Breaking this area integral and evaluating it results to an area moment of inertia for a rectangular beam with cross-section used in equation 1.



Fig. 4: Illustration of moment of inertia of a cantilever beam with uniform thickness.

The numerical model in this paper, implemented in MATLAB, modifies equation 2 by using the analysis of surface roughness as varying heights. The length of the illustrated beam in figure 5a was subdivided equally as one slice of the cross-section, C_n as shown in figure 5b. The cross-section was decomposed into uniform dx segments that runs along the width of the beam as illustrated in figure 5c. Note that every dy segment is the value of the total thickness per dx segment. The total thickness differs depending on the (1) statistical information acquired from the microscope and (2) the calculated moment of inertia.



Fig. 5: Illustration of a (a) fixed-free cantilever beam with surface roughness represented by (b) varying cross-sectional heights. In the numerical model developed, the average moment of inertia and average cross-sectional in (c) are calculated using equation 3 and 4, respectively. The cantilever's resonant frequency is then determined using equation 5.

The pertinent equations used in the model to represent roughness as variations in the cross-sectional heights of the cantilever are also provided. Expressing the average moment of inertia that describes the beam with non-uniform thickness gives:

$$I_{ave} = \frac{1}{L} \int_0^L \int_0^b \left(\int_{hmin}^{hmax} y^2 dA \right) dw dL$$
(3)

and for the consistency of the natural frequency equation in 1, the area is expressed as:

$$A_{ave} = \frac{1}{L} \int_0^L \int_0^b f(w) \, dw dL \tag{4}$$

The newly computed I_{ave} and A_{ave} replaces the area moment of inertia and the beam's cross-sectional area of a cantilever beam natural frequency as shown in equation 5.

$$\omega'_{n} = \frac{1}{2\pi} \left(\frac{\beta_{n}}{L}\right)^{2} \sqrt{\frac{E * I_{ave}}{\rho * A_{ave}}}$$
(5)

To test the functionality of the modified equation, acquired surface roughness was integrated to the moment of inertia. This was done by assuming a cantilever beam's total thickness height to be divided into two parts namely, T_1 and T_2 as presented in figure 6.



Fig. 6: Defining thickness on an SEM image of a silicon structure after deep reactive ion etching (DRIE).

Thickness T_1 represents the portion of silicon with surface roughness and varies depending on the maximum height value of the captured image. Meanwhile, thickness T_2 represents the silicon beam without roughness, with a value that is approximately 100 µm. Then, the material properties of the silicon beam that was acquired from COMSOL's material library was set as well as its boundary conditions for a fixed-free cantilever beam. Finally, the natural frequency of a cantilever beam incorporated with roughness was computed in MATLAB using equation 5.

3. Comparison of Numerical Model with FEM Simulations

To verify the numerical model developed, multiphysics model of a cantilever beam with surface roughness was simulated through FEM in COMSOL. Eigenfrequency and frequency domain analysis were performed to determine the natural frequency of the cantilever with surface roughness. A comparison was made between the analytical model and FEM simulations. Figure 7 shows the comparison between the numerical model and FEM simulations for five 100 μ m-thick cantilever beams with roughness characteristics as shown in figure 1.



Fig. 7: Surface roughness vs resonant frequency plot of a 100µm -thick silicon cantilever for both numerical model calculations and FEM simulations. Data point shows that the resonant frequency increases with surface roughness. The resonant frequency calculated using the numerical model shows about 1% error from the FEM simulations for all samples.

The first cantilever was set to have no roughness and serves as the ideal sample. For this cantilever, the analytical model gives a natural/resonant frequency of 5815.4 Hz while FEM simulation gives a resonant frequency of 5879.9 Hz, showing a 1% difference between the two methods. The other four cantilevers were incorporated with roughness by having the midline of each sample roughness in figure 1 to be exactly at the 100 μ m height of each beam as illustrated in figure 6. This was done to ensure each of the four cantilevers will have the same geometric (length, width and height) and material properties. In this way, the change of roughness can be evaluated fairly. The numerical model calculations consistently show around 1% error compared to FEM simulations. The resonant frequency is also observed to increase along with surface roughness. As the roughness increases, the farther the beam frequency is from its designed resonant frequency. Analysis indicates that an approximately 1.5 μ m *S*_q, roughness, deviates the frequency to 308.31 Hz from the ideal frequency of the beam with dimensions 5120 x 1280 x 100 μ m³.

4. Conclusion

A numerical model to determine the natural frequency of a beam with surface roughness was developed. This was done by treating the varying heights across the length of the beam as rectangular regions where moment of inertia is calculated. A simple triple integration of these rectangular region gives the moment of inertia of the beam with roughness. Along with surface roughness, this model also incorporates the device properties of the beam to predict its natural/resonant frequency. The numerical model discussed in this paper can be used to predict surface roughness effects on the resonant frequency of a cantilever beam prior to fabrication. In doing so, adjustments on the design of the MEMS device can be made in order to handle surface roughness effects. Not only that, the numerical model can also be used to determine tolerances with regards to surface roughness, which can be beneficial in designing a device's fabrication process. The numerical model can be further expanded to include surface roughness effects on other energy harvester structures which offers better average strain to increase output power for energy harvesting applications.

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