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Comprehensive Mass Resolution Model for 2D Nanomechanical Resonant Sensors

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Summary: Nanomechanical resonators have been explored as candidates for various sensing applications. Two-dimensional (2D) nanomechanical resonators are of particular interest due to their ultralow mass and large surface-to-volume ratio, which may enable high mass resolution under vacuum conditions. However, a comprehensive model for calculating dynamic range (DR) and mass resolution in 2D circular nanomechanical resonators is still lacking. In this work, we establish such a model by incorporating the effects of fringing fields and the Casimir effect. Our results indicate that fringing fields have significant impact on simulating device properties. The Casimir effect could be of relevance for low initial strain membranes and initial electrode gaps below 100 nm.

Keywords: Theoretical models, Nanomechanical resonant sensors, Dynamic range (DR), Mass resolution

Background, Motivation and Objective

Nanomechanical resonators have been investigated for sensing applications such as temperature, mass, and gas detection, due to their fast response and potential for high resolution in controlled environments like vacuum [1]. Mass changes, for example, are detected through shifts in resonance frequency [2], as illustrated in Fig. 1(c). Two-dimensional (2D) nanomechanical resonators are particularly interesting due to their ultralow mass and high surface-to-volume ratio, making them highly sensitive to external stimuli like strain, mass, light, and temperature [1]. For sensing applications, the frequency resolution (or equivalent mass resolution) is critical as it directly impacts the performance of the resonant sensor. The frequency resolution strongly depends on the dynamic range (DR), as a higher DR improves the signal-to-noise ratio (SNR) and thus allows the detection of smaller frequency shifts. In this work, we establish a comprehensive dynamic range model for circular 2D nanomechanical resonators by incorporating both the fringing fields and the Casimir effect. The model suggests that these effects may influence dynamic range and mass resolution, especially at high DC gate voltages. A parameter sweep of thickness, radius, and initial gap distance analyzes their impact, providing a framework for improved modeling of sensing performance and 2D resonant membrane design.

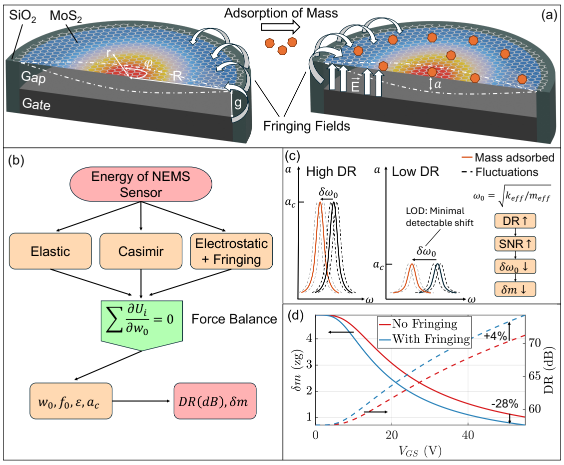

Fig. 1: (a) Schematic of mass adsorption on a resonant sensor. (b) Flowchart of the theoretical model. (c) Illustration of the minimal detectable frequency shift due to mass adsorption for sensors with low and high DR. (d) Impact of the fringing fields effect on mass resolution and DR as a function of applied gate voltage.

Theoretical Model

The resonant membrane, as seen in Fig. 1(a), is capacitively actuated by DC and AC voltages. Properties such as static center deflection (w_0), strain (ε), resonance frequency (f_0), and critical amplitude (a_c) are derived from the force balance, obtained by differentiating the total system energy (Fig. 1(b)). The electrostatic energy (including fringing fields [3]) and Casimir energy [4] contributions are given by:

$$U_{es} = \frac{\pi \varepsilon_0 R^2}{2w_0} \ln\left(\frac{g}{g-w_0}\right) V_{GS}^2 A_f\,, \qquad (1)$$

$$A_f = 1 + c_1 \frac{g}{R} + c_1 \frac{g}{R} \ln\left(\frac{c_2 R}{g}\right), \qquad (2)$$

$$U_{cs} = \eta_0 \frac{\pi^3 \hbar c R^2}{1440 w_0} \left(\frac{1}{(g-w_0)^2} - \frac{1}{g^2}\right), \qquad (3)$$

where R is radius, g is gap distance, A_f is the fringing fields factor, c_1 and c_2 are fitting parameters, and η_0 is the Casimir factor (accounting for the conductivity of the materials). From the derived properties, the DR and the mass resolution are determined by [5]:

$$\text{DR} = 20\log\left(\frac{0.745a_c}{\sqrt{2S_{x,th}\Delta f}}\right), \qquad (4)$$

$$\delta m \approx \frac{2m_{eff}}{Q} \times 10^{-\text{DR (dB)}/20}, \qquad (5)$$

where $S_{x,th}$ is thermomechanical noise, Δf is measurement bandwidth, m_{eff} is effective mass, and Q is quality factor. The DR describes the ratio between the maximum vibration amplitude and the noise floor, reflecting the signal-to-noise ratio. A higher DR thus enables the detection of smaller masses.

Results and Discussion

According to our model, the Casimir effect begins to influence the device properties only when the gap distance is below 100 nm, the initial strain is low, and the applied voltage is small or zero. In all other cases, its effect is negligible. To investigate the effect of fringing fields on resonant sensor performance, we sweep the DC gate voltage and evaluate the resulting dynamic range and mass resolution, as shown in Fig. 1(d). The calculated DR and mass resolution are higher when fringing fields are taken into account. Notably, the impact of the fringing fields effect is primarily governed by the device's radius-to-gap ratio (R/g), with the model showing a 4% increase in DR observed for R/g = 1 at 50 V, reaching up to 73 dB. This corresponds to an approximately 28% lower minimal detectable mass, reaching sub-zeptogram levels for a device with R=0.5μm and t=2nm. Moreover, at higher DC gate voltages, the difference between models with and without fringing fields becomes more pronounced.

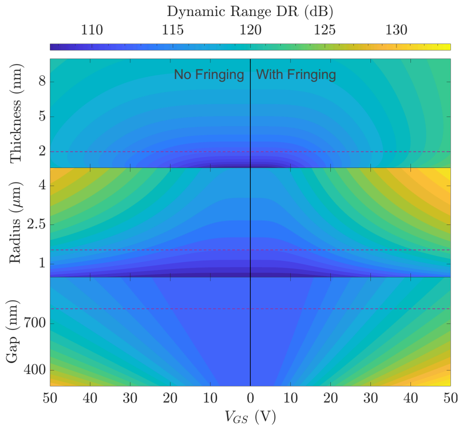

Fig. 2: Dynamic range as a function of varying geometric device parameters: (a) thickness, (b) radius, and (c) gap. The fringing fields effect is considered for the right side of the plot. The purple lines represent the fixed parameter values.

To better visualize how geometric device parameters influence the DR and how fringing fields affect it, Fig. 2 presents a parameter sweep with and without considering the fringing fields effect. We observe, that when fringing fields are considered the DR increases faster with applied gate voltage. Additionally, DR increases with increasing radius and decreasing gap distance, while an increase in thickness enhances DR at low voltages but reduces it at higher voltages. Similarly, Fig. 3 presents the parameter sweep for mass resolution. Since mass resolution is directly derived from the DR, it exhibits the same trends observed for DR.

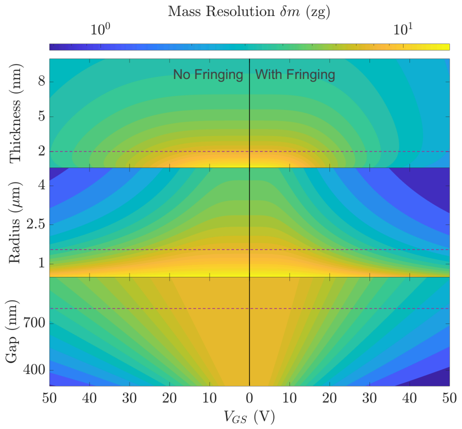

Fig. 3: Mass resolution as a function of varying geometric device parameters: (a) thickness, (b) radius, and (c) gap. The fringing fields effect is considered for the right side of the plot. The purple lines represent the fixed parameter values.

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