Modeling and simulation of a ZnO nanowire bridge and development of an electrical equivalent circuit in liquid

Ritu Bajpai and Mona Zaghloul
Department of Electrical and Computer Engineering
The George Washington University
Washington DC, USA
ritu_ece@gwu.edu

***Abstract*—This paper presents the modeling and simulation of ZnO nanowire bridge and its application as a mass sensor. The resonant frequency shift due to added mass has been used as the sensing parameter. The finite element modeling (FEM) analysis results of the resonant frequency computation conform to the theoretical results within an error of 3%. An electrical equivalent circuit of the bridge structure has been proposed for the operation of the device in liquid. The simulated frequency response of the equivalent circuit matches the theoretical results.**

I. INTRODUCTION

FEM analysis tools have been used before for studying the response of nanowire resonators. [1] and [2] show the modeling of nanowire cantilever structure using FEM technique. In this paper a ZnO nanowire bridge has been modeled using commercially available FEM modeling tool COMSOL [3]. The bridge is supported by electrodes at the two ends which are also used for device actuation. Change in resonant frequency of the bridge with addition of mass to the structure can be used for sensing applications. Integration of such MEMS based sensing devices with read out electronic circuitry [4] promises device miniaturization and System-On-Chip (SoC) design. This leads to a need for simulating together the MEMS and the electronic circuitry together for design purposes. One way to accomplish this is formulation of an equivalent circuit model for the MEMS structure. An equivalent circuit model allows the use of standard circuit simulation softwares for device analysis. We developed the equivalent circuit model for ZnO nanowire bridge with similar actuation electrode geometry in [5]. However, this model is not applicable for device operation in liquid. This is a drawback because mass sensors are useful in biological applications where there is often a need to operate them in liquid [6, 7].

In this paper, the equivalent circuit of the device presented in [5] has been extended to represent the response of the device in liquid. When the device is submerged in liquid, the resonant frequency is reduced along with a decrease in quality factor and signal amplitude. Therefore when beam structure is designed to operate in liquid we need to amplify its response for improved performance. Reference [8] and [9] present techniques for improved response of the device in liquid. Formulation of an equivalent circuit makes it possible to simulate the device with essential circuitry for improved performance using circuit simulation softwares.

II. FEM MODELLING OF THE BRIDGE STRUCTURE

ZnO nanowire is modeled as a bridge supported at two ends. This is similar to the case of a fixed-fixed beam in vibration mechanics. To simplify the model, the nanowire used in this section is assumed to have a square cross-section. The beam is 1 um in length and 100 nm in width and thickness. The analysis was performed using multiphysics computational tool COMSOL [3].

A. *Modal Analysis*

Fig. 1 shows the lowest four modes of vibration for the beam when it is actuated with a dc voltage applied across it. Mode 1, 2 and 4 are the flexural modes while mode 3 is the torsional modes of vibration. Resonant frequency, f for flexural mode of vibration can be theoretically estimated as [10]

$$f_n = \frac{\eta_{n,b}^2}{\sqrt{3}\pi}\sqrt{\frac{E}{\rho_b}}\frac{t}{L^2} \qquad (1)$$

Here n denotes the mode of vibration, E is the Young's modulus (119.7 GPa), ρ_b is the density of the material of the beam (5680 kg/m^3) [3], t and L are the thickness and the length of the beam respectively. $\eta_{n,b}$ is a constant whose value for the first 3 modes of vibration is [10]

$$\eta_{1,b} = 2.365$$

$$\eta_{2,b} = 3.927$$

$$\eta_{3,b} = 5.498$$

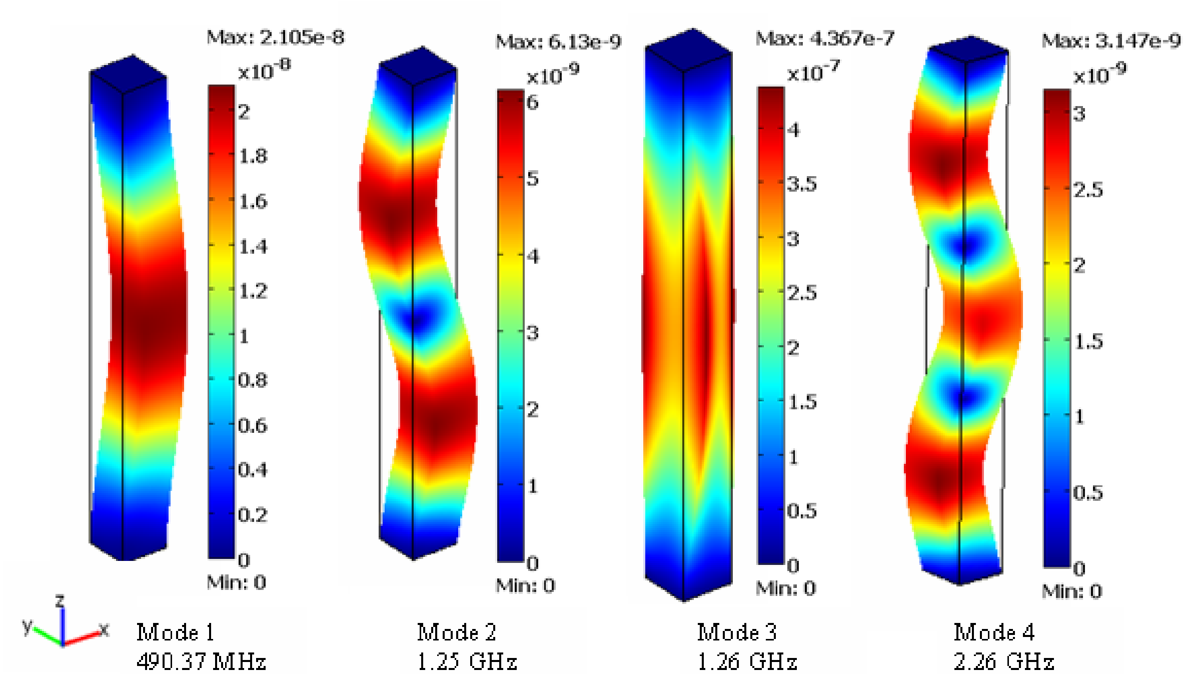

Figure 1. Lowest four mode shapes and displacement contour of a ZnO nanowire with a fixed-fixed beam boundary condition. Maximum displacement in m.

From FEM simulation, the resonance frequency of the first mode of vibration is found to be 490.37 MHz. The calculated frequency using (1) gives an error of 3% from the simulated results.

B. *Harmonic Analysis*

The harmonic analysis plot gives the frequency response of the structure with the input signal frequency. Fig. 2 shows the fundamental resonant frequency for the point at the center of the beam. From Fig. 2, the resonant frequency of the first mode of vibration is found to be 490.37 MHz, same as that obtained from the modal analysis.

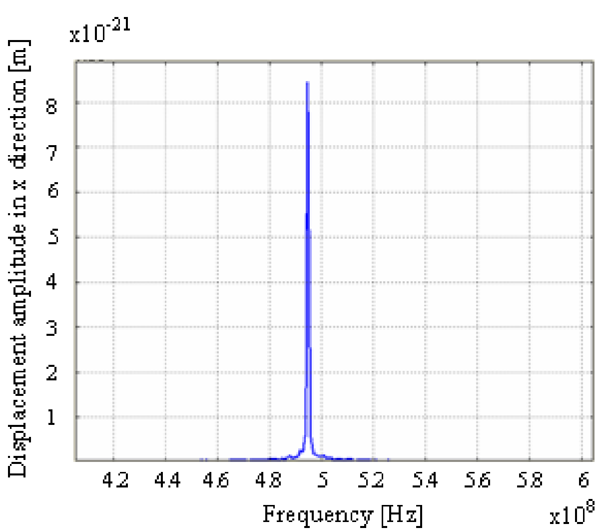

Figure 2. Harmonic response of the beam at the point in the centre of the beam.

III. BRIDGE STRUCTURE AS A MASS SENSOR

Equation (1) can be re-written as (3) in terms of the force constant *k* and the mass *m* of the system giving the frequency and the mass relationship of the bridge structure.

$$f = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \qquad (2)$$

This suggests that for an additional mass deposited on the nanowire, we should observe a shift in the fundamental resonant frequency. Differentiating (3) we obtain

$$\frac{\Delta f}{f} = -\frac{1}{2}\frac{\Delta m}{m} \qquad (3)$$

where Δm is the mass added to the nanowire and Δf is the frequency shift. The negative sign indicates that the resultant fundamental resonant frequency is less than the frequency of the unloaded nanowire. To study this, the frequency response was studied with additional external mass distributed uniformly on the surface of the bridge. The sensitivity of the mass sensor is defined as the change in frequency with change in mass of the structure, $\Delta f/\Delta m$. From (4) we see that the sensitivity of the sensor is proportional to the resonant frequency of the bridge. Therefore, higher sensitivity can be achieved by using higher modes of vibration. The analysis in this section has been performed for the fundamental flexural resonant frequency for a beam with length 1 um and width and thickness of 100 nm each.

For a 1 nm thick uniform layer of gold deposited on the top surface of the beam, the change in mass $\Delta m = 1.93 \times 10^{-15}$ g. From (4) we obtain the shift in frequency Δf=8.33 MHz and

FEM analysis yields $\Delta f = 9.35$ MHz. The frequency shift Δf is found to be linear w.r.t to mass loading from the simulation study which is in accordance with (4).

IV. ELECTRICAL EQUIVALENT CIRCUIT

Lumped modeling of the piezoelectric devices is a standard approach for simplified device representation [11]. The electrical equivalent circuit of the given structure as shown in Fig. 3 has been derived in [5]. From Fig. 3 we see that the device equivalent circuit has two branches. One branch containing C_0, contributes to the static capacitance arising from the electrodes located on the opposite ends of the ZnO nanowire. This capacitance dominates the admittance away from resonance. The other branch containing elements which dominate the admittance near resonance is called the motional branch of the circuit. C_e, L_e and R_e are the motional capacitance, inductance and resistance respectively. In the equivalent circuit the vibrating mass of the crystal is represented by the motional inductance, L_e. The elasticity of the piezoelectric material is represented as a motional capacitance, C_e, and the mechanical losses are represented by an equivalent motional resistance, R_e. The values of various electrical components are given by [5]

$$C_0 = \varepsilon_{33}\left(\frac{tb}{L}\right) \tag{4}$$

$$C_e = C_{11} d_{31}^2 \left(\frac{tb}{L}\right) \tag{5}$$

$$L_e = \frac{m^*}{n^2} \tag{6}$$

$$R_e = \frac{m^* \omega}{Qn^2} \tag{7}$$

Here t, b and L are the thickness, width and the length of the beam respectively. ε_{33}, C_{11}, d_{31} are the permittivity in z direction, stiffness coefficient and piezoelectric stress coefficient of ZnO respectively. n is the electrical to mechanical transformer ratio, ω is the frequency in radians per seconds given by $2\pi f$. m^* is the effective mass of the system expressed as

$$m^* = \frac{k}{\omega^2} \tag{8}$$

k is the spring constant of the system.

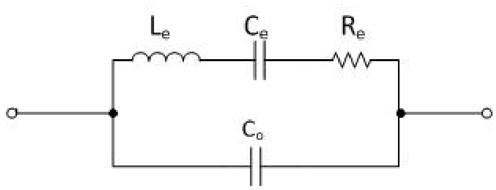

Figure 3: Equivalent circuit of a nanowire bridge structure.

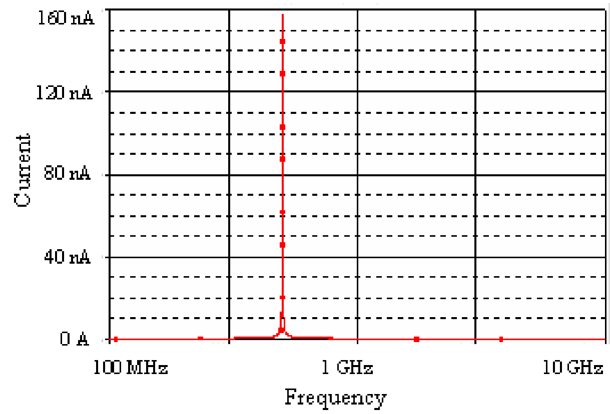

Figure 4. Frequency response of the electrical equivalent circuit.

Frequency response of the equivalent circuit has been plotted in Fig. 4.

The percentage error in the fundamental resonant frequency obtained from FEM analysis of the mechanical structure and that obtained from the equivalent circuit response is 1.33%.

V. EQUIVALENT CIRCUIT IN LIQUID

Due to large sensing application of nanowire mechanical structures, there is often a need to operate these devices in liquid. In this case the electrical equivalent circuit derived in previous section is not the correct representation of the device. To incorporate the influence of the surrounding liquid in the electrical equivalent circuit we need to consider the additional forces that are now acting on the beam. In [12], vibrational behavior of the doubly clamped beam immersed in liquid has been investigated. Influence of the surrounding liquid on the vibrating beam has been accounted for by adding respective resistance terms to the harmonic beam equation. The interaction of the beam with the viscous fluid can be accounted for by adding a viscous damping term and an added mass term to the Bernoulli-Euler beam equation [13]. The mass term accounts for the mass of the fluid which is dragged along with the beam and acts like an added mass to the structure. The viscous damping term accounts for the pressure exerted by the surrounding fluid on the faces of the beam and the friction introduced due to the liquid.

The equivalent circuit model derived in the previous section has been extended to be applicable for operation of the device in liquid based on the analysis presented in [12]. The harmonic fluid resistance, k' can be interpreted as the real part k_m, representing an added mass coefficient and the imaginary part k_d, representing the damping coefficient. The expression for k' is given by

$$k'(\omega) = (k_m - jk_d)\pi\rho_l b'^2 \omega^2 \tag{9}$$

Where b', ρ_l and j are the half beam width $b/2$, density of the fluid and the imaginary unit respectively.

The values of k_m and k_d depend on the Reynolds number R, of the fluid which can be expressed as

$$R = b'^2 \omega \frac{\rho_l}{\mu} \quad (10)$$

Here μ is the viscosity of the fluid.

Now k_m and k_d can be evaluated using the polynomial fitting method to give

$$k_m \approx \frac{2.8}{\sqrt{R}} + 1 \quad (11)$$

$$k_d \approx \frac{4.4}{\sqrt[3]{R^2}} + 0.065 \quad (12)$$

For simplicity, we consider the surrounding fluid to be water with density 1000 kgm^{-3} and viscosity 8.9x10-4 $kgm^{-1}s^{-1}$ which gives R as 8.65. We can now calculate the corresponding value of the added mass and damping coefficients by substituting R in (11) and (12) which yields k_m= 1.68 and k_d=1.10. The values for k_m and k_d have also been analytically computed in [14] which yield results similar to those obtained from (11) and (12).

Using k_m and k_d we can now determine the new resonant frequency of the device in liquid. The resonant frequency in radians per second, of the beam in nth mode, immersed in liquid, ω_l is given as [12]

$$\frac{\omega_l}{\omega} = \left[1 + \kappa\left(k_m + k_d^2 \frac{1}{k_m + \kappa^{-1}}\right)\right]^{-\frac{1}{2}} \quad (13)$$

where

$$\kappa = \frac{\pi \rho_l b}{4 \rho_b t} \quad (14)$$

Substituting the values in (13) and (14) we get the fundamental resonant frequency as 438.5 MHz.

Similarly the quality factor of the device in liquid can be computed as [12]

$$Q' = \left[\sqrt{1 + \frac{k_d}{k_m + \frac{1}{\kappa}}} - \sqrt{1 - \frac{k_d}{k_m + \frac{1}{\kappa}}}\right] \quad (15)$$

As we see from (4-7), the capacitance terms in the equivalent circuit model depend only on the physical dimensions of the device and its material properties and hence remain unchanged for the equivalent circuit model in the liquid. On the other hand, the inductance and the resistance terms depend on the frequency, quality factor and the effective mass of the device. Therefore the effect of the surrounding liquid will be accounted for by adding an extra inductance, L_1 and resistance, R_1 to the equivalent circuit as shown in Fig. 5.

From (8) and (13) we get the effective mass of the device in liquid as

$$m' = \frac{k}{\omega_l^2} \quad (16)$$

If m_f is the effective added mass due to the fluid

$$m' = m^* + m_f \quad (17)$$

L_1 is the inductance due to the added mass m_f to the device and is evaluated using (6). Modified resistance of the equivalent circuit is computed by substituting the modified values of frequency, effective mass and quality factor of the system in (7). Added resistance due to the surrounding liquid, R_1 is the difference of the modified resistance and the resistance R_e.

$$L_1 = \frac{m_f}{n^2} \quad (18)$$

$$R_1 = \frac{m' \omega_l}{Q' n^2} - R_e \quad (19)$$

Fig. 6 shows the frequency response of the modified equivalent circuit. The frequency has shifted to 453.32 MHz, differing less than 3.4% from the frequency computed from (13).

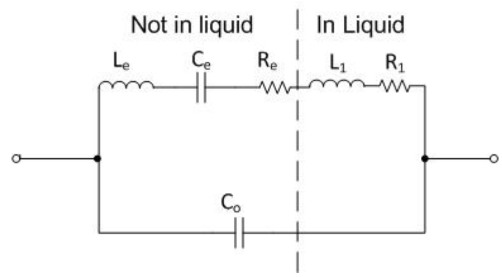

Figure 5. Electrical equivalent circuit of the device in liquid.

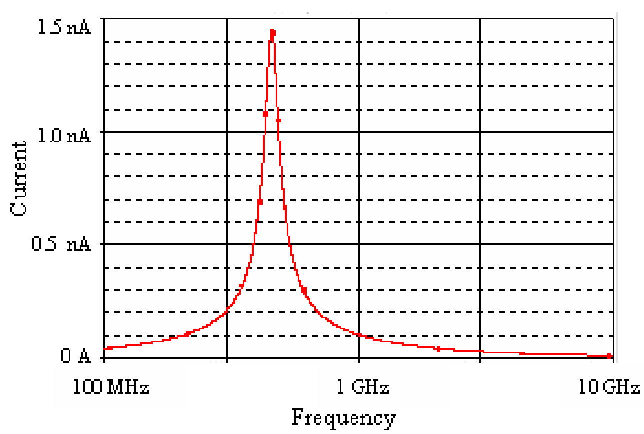

Figure 6. Frequency response of the electrical equivalent circuit of the device in liquid.

VI. CONCLUSION

In this paper we modeled the ZnO nanowire bridge structure for the mass sensing application. Equivalent circuit of the device proposed earlier has been extended to develop an equivalent circuit model of the device operating in liquid. The frequency response of the model has been verified to give the modified values of frequency and quality factor as analytically proposed elsewhere.

Biological application of nano scale mass sensors often requires operation in liquid environment which leads to deteriorated output response. Such modeling of the structure in equivalent circuit form will enable us to design with standard circuit simulation tools, the essential read out circuitry for improvement of the output response. Design of the read out circuitry integrated with the equivalent circuit model can be an interesting future study derived from this work.

REFERENCES

[1] R. Bajpai, O. Tigli and M. Zaghloul, "Modeling and simulation of a nanowire-based cantilever structure" Proceedings of EuroSimE 2009, pp. 1-4.

[2] W. Lee, M. Jeong and J. Myoung, "Fabrication and application potential of ZnO nanowires grown on GaAs(002) substrates by metal\–organic chemical vapour deposition" Nanotechnology 15(3), pp. 254-259, 2004.

[3] www.comsol.com

[4] A. Uranga, N. Barniol, H. Campanella, J. Esteve, L. Teres and Z. Davis, "A read-out strategy and circuit design for high frequency MEMS resonators" Circuits and Systems, 2005. ISCAS 2005. IEEE International Symposium on pp. 5361-5364 Vol. 6.

[5] R. Bajpai and M. Zaghloul, "Modeling a fixed-fixed beam nano biosensor using equivalent electrical circuit technique" Life Science Systems and Applications Workshop, IEEE/NIH pp. 58-61, 2009.

[6] Hao Zhang, M. S. Marma, Eun Sok Kim, C. E. McKenna and M. E. Thompson, "Implantable resonant mass sensor for liquid biochemical sensing", 17th IEEE International Conference on Micro Electro Mechanical Systems (MEMS) pp. 347-350, 2004.

[7] J. Weber, W. M. Albers, J. Tuppurainen, M. Link, R. Gabl, W. Wersing and M. Schreiter, " Shear mode FBARs as highly sensitive liquid biosensors", Sensors and Actuators A: Physical 128(1), pp. 84-88, 2006.

[8] J. Tamayo, A.D.L. Humphris, A.M. Malloy and M.J. Miles, "Chemical sensors and biosensors in liquid environment based on microcantilevers with amplified quality factor", Ultramicroscopy 86(2001) 167-173.

[9] A. Vidic, D. Then and Ch. Ziegler, "A new cantilever system for gas and liquid sensing", Ultramicroscopy 97 (2003) 407-416.

[10] D. S. Greywall, "Micromechanical RF filters excited by the lorentz force", J Micromech Microengineering 9(1), pp. 78-84, 1999.

[11] Stephen D. Senturia, Microsystem Design,Kluwer Academic Publishers, 2001.

[12] B. Weiss, E. K. Reichel and B. Jakoby, "Modeling of a clamped–clamped beam vibrating in a fluid for viscosity and density sensing regarding compressibility" Sensors and Actuators A: Physical 143(2), pp. 293-301, 2008.

[13] Erwin K. Reichel1, Bernhard Weiß, Christian Riesch, Artur Jachimowicz, Bernhard Jakoby,"A novel micromachined liquid property sensor utilizing a doubly clamped vibrating beam" *Eurosensors XX Proceedings 2006, in Eurosensors*, Vol. 1, 9-2006.

[14] E. O. Tuck, "Calculation of unsteady flows due to small motions of cylinders in a viscous fluid" J Eng Math 3(1), pp. 29-44, 1969.