GENERALIZED MACHINE LEARNING METHOD TO EXTRACT FREQUENCY-COMPLIANCE COEFFICIENTS FROM MEMS RESONATOR MODEL

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ABSTRACT

Micromachined resonators, essential for modern timekeeping devices, are a subset of MEMS components. The focus here is on capacitive resonators with electrostatically driven micro-beams, where voltage induces mechanical vibration. Resonant frequency is sensitive to temperature changes, governed by material elastic properties. Modeling this dependence is crucial for engineers to compensate accurately. We extracted coefficients linking elastic properties to resonant frequency using multivariable Taylor expansion as our ML model. Our approach is generalized beyond capacitive resonators to include piezoelectric resonators, and our LCR model can adapt with experimental or finite element data available in the future. Future work could extend our model to incorporate temperature dependence.

KEYWORDS

Microelectromechanical systems, resonators, lumped element, taylor series, machine learning

INTRODUCTION

Micromachined resonators, known for their applications in modern timekeeping devices, are an important subset of MEMS (Microelectromechanical Systems) components [1]. The type of resonators focused on this investigation are capacitive resonators which consists of electrostatically driven micro-beam (Fig. 1), where voltage across electrodes induce a mechanical vibration in the beam and vice versa [2,3].

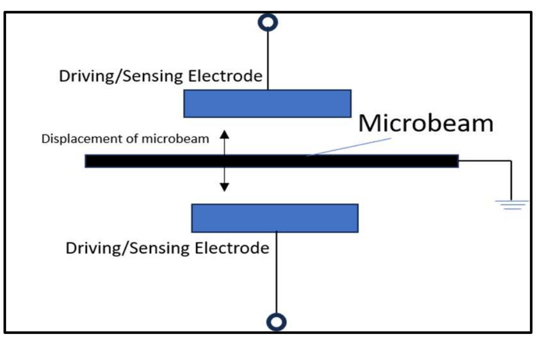

Figure 1: Simplified diagram depicting the structure of a MEMS resonator

Acknowledging that the resonant frequency is sensitive to changes in temperature and that temperature dependence is governed by the materials elastic properties', it is important to be able to model the dependence between the resonant frequency of the resonator and the elastic properties to allow engineers to precisely compensate for the dependencies [4].

In this work, we aim to extract the coefficients of the model that relates the resonators' elastic properties to its resonant frequency using the multivariable Taylor expansion as our machine learning (ML) model differing modes of vibration. Ng E.J. et al [4] used a traditional curve fitting method based on their training dataset from finite element analysis to extract the frequency-compliance coefficients. Here, we use the inductance-capacitance-resistance (LCR) model in order to map it to the resonator system and generate our training data based on simulation. We then use this training dataset to train our ML model which is derived in the methodology and validate its accuracy (using training data that was not shown to the model).

Moreover, while they modeled the dependence for capacitive resonators, our work focuses on a more generalized model applicable to other forms of resonators like piezoelectric resonators. The main model used to model the system is the inductance-capacitance-resistance (LCR) model, which gives us the advantage of seamless integration with experimental or finite element analysis data.

METHODOLOGY

The methodology is divided into 3 phases: Model Development, Training Data Generation, Training the model. For the first 2 phases, the figure 2 below summarizes how the flow of the work looks like.

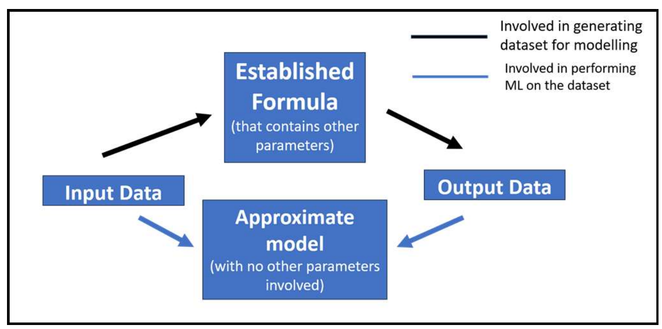

Figure 2: Flow of methodology

Developing the Model

The overview behind the mathematical foundations of the model is shown in the following explanation. To derive the dependence, a lumped element circuit can be used to model the LCR system. LCR system is composed of an inductance component, capacitance component and resistance component as shown in Figure 3 below.

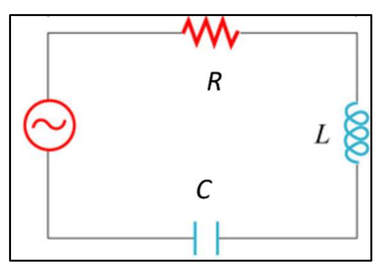

Figure 3: LCR Circuit Model [5]

Our resonator system has the same second order differential equations describing the LCR system as such: $\ddot{q} + \frac{R}{L}\dot{q} + \omega_0^2 q = \frac{V_0}{L}cos(\omega t)$ from ref. [6] where $\omega_0^2 = \frac{1}{LC}$ and q is charge, R is resistance, L is inductance, V_0 is driving voltage. The solution for this differential equation is:

$$A = \frac{\frac{V_0}{L}}{\sqrt{(\omega_0^2 - \omega^2)^2 + \omega^2(\frac{R}{L})^2}} \tag{1}$$

where A is the amplitude of complex charge as modelled (Fig. 4) below (with the values of parameters given in table 1 further below).

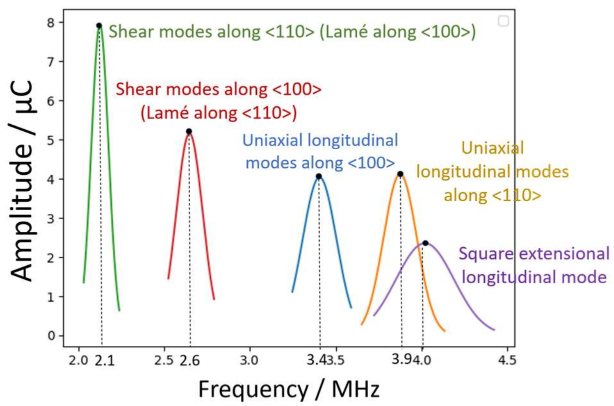

Figure 4: Amplitude for different frequencies. The same value of $\frac{R}{L}$ was used for all modes, obtained from Ref. [7]

Given that $\omega_0{}^2 = \frac{1}{LC}$ in the LCR model [8] which is equivalent to $\omega_0{}^2 = \frac{k}{m}$ [9] in a spring-mass-damper model (where k is the spring constant and m is mass) along with the fact that $\omega_0 = 2\pi f$ from ref. [9] , rewrite f(resonant frequency) as:

$$f = \frac{1}{2\pi}\sqrt{\frac{k}{m}} = \frac{1}{l_{eff}}\frac{1}{\sqrt{\rho s_{eq}}} \tag{2},$$

where l_{eff} is the effective length of the resonator (metres), ρ is density of the resonator ($kg\,m^{-3}$), s_{eq} is the equivalent compliance (Pa^{-1}) of the system.

The fractional frequency dependence on the fractional equivalent compliance can be derived from (2) to yield the following equation [4]:

$$\frac{\Delta f}{f} \approx -\frac{1}{2}\left(\frac{\Delta s_{eq}}{s_{eq}}\right) + \frac{3}{8}\left(\frac{\Delta s_{eq}}{s_{eq}}\right)^2 \tag{3}$$

The fractional equivalent compliance $(\frac{\Delta s_{eq}}{s_{eq}})$ in equation (3) can be modeled using multivariable Taylor expansion to relate it with 3 independent components of the compliance (s_{11}, s_{12}, s_{44}) as shown in equation (4.1) below. Although an expansion to the second order is possible, it is only done up to the first order because of the nature of the linear relationship between equivalent compliance and its 3 independent components in the modes of vibration that are considered. Note that the variable i in equation (4.1) below indexes through the 3 independent components: {11,12,44}.

$$\frac{\Delta s_{eq}}{s_{eq}} = \sum_i (\mu_i)\left(\frac{\Delta s_i}{s_i}\right) \text{ where } \mu_i = \frac{\partial\frac{\Delta s_{eq}}{s_{eq}}}{\partial\frac{\Delta s_i}{s_i}} \tag{4.1}$$

Given that $s_{eq} = \sum_i \lambda_i(s_i) = \lambda_{11}s_{11} + \lambda_{12}s_{12} + \lambda_{44}s_{44}$, where s_{eq} is linearly related to the 3 independent components by the corresponding coefficients, λ_i obtained from Ref. [10], the first order Taylor expansion of $\frac{\Delta s_{eq}}{s_{eq}}$ in equation (4.1) will simplify (from ref. [4]) to:

$$\frac{\Delta s_{eq}}{s_{eq}} = \sum_i \left(\lambda_i\left(\frac{s_i}{s_{eq}}\right)\right)\left(\frac{\Delta s_i}{s_i}\right) \tag{4.2}$$

Substituting equation (4.2) into equation (3) yields equation (5) from Ref. [4]:

$$\frac{\Delta f}{f} \approx -\frac{1}{2}\left(\frac{\Delta s_{eq}}{s_{eq}}\right) + \frac{3}{8}\left(\frac{\Delta s_{eq}}{s_{eq}}\right)^2 \approx \sum_i \gamma_i\left(\frac{\Delta s_i}{s_i}\right) + \sum_i\sum_j \gamma_{i,j}\left(\frac{\Delta s_i}{s_i}\right)\left(\frac{\Delta s_j}{s_j}\right) \tag{5}$$
$$where\ \gamma_i = -\frac{1}{2}\lambda_i\left(\frac{s_i}{s_{eq}}\right)\ and\ \gamma_{i,j} = \frac{3}{8}\lambda_i\lambda_j\left(\frac{s_i}{s_{eq}}\right)\left(\frac{s_j}{s_{eq}}\right)$$

Equation (5) is thus the approximated model that we will be using and the γ_i and $\gamma_{i,j}$ coefficients are the coefficients that we will try to extract using machine learning.

Training Data Generation

For the machine learning model however, we need a training data set with input and output data to perform ML on. To generate the training data, $\frac{\Delta s_i}{s_i}$ will be varied from -1% to 1% for each of the individual components which is actually based on the expected variation due to temperature changes [4].

Using equation (5) with the corresponding coefficients of the particular mode of vibration, s_{eq} will be calculated for a particular instance. This allows us to make use of the established formula in equation (2), with the necessary parameters, to output frequency data. Thus, effectively producing training data that can be used to train the ML model. The workflow described above is summarised with the workflow in figure 5 below.

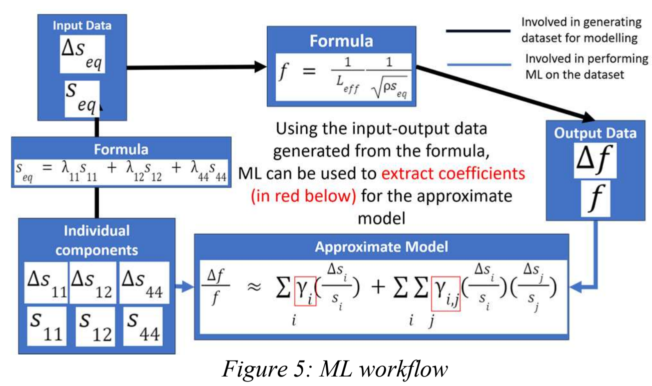

Figure 5: ML workflow

To generate data from formula (2), we would need the values for the following parameters: $\boldsymbol{l_{eff}}$, $\boldsymbol{\rho}$, $\boldsymbol{s_{eq}}$. The value of seq can be calculated using $\boldsymbol{s_{eq} = \sum_i \lambda_i(s_i)}$ where the values of $(\boldsymbol{s_{11}, s_{12}, s_{44}})$ would be required. The values of the necessary parameters and variables are summarized in the table below.

Table 1: Table of parameters

Parameter	Unit	Value	Ref.
l	μm	1089	[12]
ρ	$kg\ m^{-3}$	2330	[13]
$\{s_{11}, s_{12}, s_{44}\}$	10^{-12} Pa^{-1}	$\{7.8, -2.2, 12.9\}$	[4]
V_0	V	1	[7]
L	H	0.244	[7]
R	$k\Omega$	1.24	[7]

Model Training

Using the methodology described in the previous section, training data is generated using a self-written python code. ML is then performed on the training data by the model stated in equation (5). To check the validity of the model, the ML model is evaluated with the coefficient of determination, R^2, which is a well established statistical measure of the variation in the predicted variable [11].

FINDINGS

The table below contains the extracted coefficients of the model that relates the resonators' elastic properties to its resonant for the specific modes of vibration - Uniaxial longitudinal modes along <100>, Uniaxial longitudinal modes along <110>, Shear modes along <110> (Lamé along <100>), Shear modes along <100> (Lamé along <110>), Square extensional longitudinal mode.

Table 2. Table summarizing the different frequency-compliance coefficients extracted from model

Resonant Mode	Modeled frequency-compliance coefficients			R^2 value
	γ_{11} γ_{12} γ_{44}	$\gamma_{11,12}$ $\gamma_{12,44}$ $\gamma_{11,44}$	$\gamma_{11,11}$ $\gamma_{12,12}$ $\gamma_{44,44}$	
Uniaxial longitudinal modes along <100>	-0.502 0 0	0 0 0	0.377 0 0	0.99999 7
Uniaxial longitudinal modes along <110>	-0.325 0.092 -0.269	-0.045 -0.037 0.131	0.158 0.012 0.108	0.99999 5
Shear modes along <110> (Lamé along <100>)	-0.391 -0.11 0	0.065 0 0	0.229 0.018 0	999998
Shear modes along <100> (Lamé along <110>)	0 0 -0.5	0 0 0	0 0 0.375	0.99999 7
Square extensional longitudinal mode	-0.702 0.199 0	-0.209 0 0	0.737 0.058 -0.001	0.99998 1

From table 2, the approximate model developed in this paper is highly accurate in relating resonant frequency to the elastic compliance as seen from the extremely high R^2 value for each mode of vibration. The frequency-compliance coefficients that we extracted from this paper can be used to further modelling in the future. In fact, the fact that we used values from a piezoelectric resonator while relying on the model for a capacitive resonator displays the vast applicability of this model across different types of resonators. Therefore, with more available data through experimental data or finite element analysis data in the future, we can develop an even more generalised and accurate model for resonators. Moreover, the main implication of this work is to be able to relate temperature-frequency dependence. Given that we have modelled the dependence between the elastic constants and the frequency, by identifying the impact of temperature on the elastic constants, we can achieve the ultimate aim of developing the model for temperature-frequency dependence as summarised, in the future, as simply illustrated by the figure 6 below.

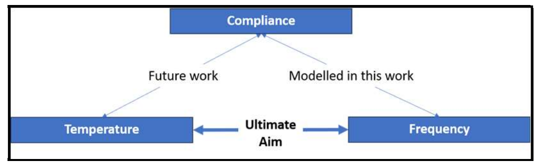

Figure 6: Future work

On another a note, while one of the main advantage of this model stems from the elegant linear combination of (s_{11}, s_{12}, s_{44}) to calculate s_{eq} for their corresponding modes of vibration, it is important to note that resonator devices can deviate away from these ideal modes of vibration due to minor geometric differences in the orientation of the resonator along with the presence of other components like supporting anchors and release-etch holes. In these cases, a finite element analysis might do a better job to account for the actual geometry of the device. However, our model provides a good starting point for such modelling purposes.

CONCLUSION

The coefficients for the frequency-compliance dependence for the model in equation (5) (restated below) was successfully extracted in this paper.

$$\frac{\Delta f}{f} \approx -\frac{1}{2}\left(\frac{\Delta s_{eq}}{s_{eq}}\right) + \frac{3}{8}\left(\frac{\Delta s_{eq}}{s_{eq}}\right)^2 \approx \sum_i \gamma_i \left(\frac{\Delta s_i}{s_i}\right) + \sum_i \sum_j \gamma_{i,j} \left(\frac{\Delta s_i}{s_i}\right)\left(\frac{\Delta s_j}{s_j}\right) \quad (5)$$

$$where\ \gamma_i = -\frac{1}{2}\lambda_i\left(\frac{s_i}{s_{eq}}\right)\ and\ \gamma_{i,j} = \frac{3}{8}\lambda_i\lambda_j\left(\frac{s_i}{s_{eq}}\right)\left(\frac{s_j}{s_{eq}}\right)$$

Using python to generate training data, and training a ML model using that data allowed us to extract coefficients for the model above. The model seems to perform quite accurately with relatively high R^2 scores. Our model can be improved even more when more experimental or finite element analysis data becomes available in the future. Moreover, another potential extension would be the incorporation of temperature dependence into our model which would act more useful for the MEMS industry.

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