Multiphysics Analysis of Thermoelastic Damping Effects on RF MEMS Components

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Abstract— Modeling and simulation of Thermoelastic Damping (TED) is an important issue in the development of RF MEMS components. TED is a critical loss mechanism in numerous high Q microstructures and induced by the irreversible heat dissipation during the coupling of heat transfer and strain rate in an oscillating system. The magnitude of the energy loss depends on the vibrational frequency and the thermal relaxation time constant of the structure. The energy dissipation mechanism highly affects the Q factor. In this paper, the effects of TED on simple fixed-fixed type beam resonators and thin film resonators are analyzed. The effects of material properties and geometry on the Q factor is analyzed in the case of simple fixed-fixed beam resonators. Depending on the resonance frequency of different structures, different Q are obtained. In the case of thin film resonators a new geometry is developed to improve Q factor by reducing TED effects. By attaching folded springs to the existing MEMS structures, the effect of temperature on eigen frequency and Q factor can be reduced to a certain extent. The folded springs relieve axial stress because it is free to expand or contract in the axial direction and sensitivity to stress is thus reduced. The different eigen mode frequencies are also reduced which accounts for the improvement in Q factor for the folded structure. Modeling and simulation of TED effect on various resonators are done by using COMSOL Multiphysics software.

Keywords- Thermoelastic damping, Eigen frequency analysis, Simple fixed-fixed beam resonators, Thin film resonators.

1 INTRODUCTION.

Thermoelastic damping has been identified as an important loss mechanism in MEMS resonators [1]-[4]. With the advent of the microelectromechanical systems (MEMS) technology, MEMS resonators with low weight, small size, low consumption energy and high durability have been extensively utilised for various sensing and wireless communications applications such as accelerometers, gyroscopes, oscillators, and filters [1].

The main advantage of MEMS resonators lies in the possible integration onto the silicon based IC platforms. Silicon MEMS resonators are positioned as potential competitors to quartz crystal resonators[5] [6]. However, to compete with the mature, well-established quartz technology, silicon MEMS resonators must first provide the same or better performance characteristics. For all these applications, it is important to design and fabricate microelectromechanical resonators with very high quality factors (Q factors) or very little energy loss. Q factor is defined as the ratio of total system energy to dissipation that occurs due to various damping mechanisms. Thermoelastic damping is considered to be one of the most important factors to elicit energy dissipation due to the irreversible heat flow of oscillating structures in the micro scales. In this study, the Q-factor for thermoelastic damping is investigated in various RF MEMS resonators, because a high quality factor directly translates to high signal-to-noise ratio, high resolution, and low power consumption. A low value of Q implies greater dissipation of energy and results in reduced sensitivity, degraded spectral purity and increased power consumption [7]. It is therefore desirable to eliminate, or mitigate, as many mechanisms of dissipation as possible.

Various energy dissipation mechanisms exist in microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS) [6]. Several different mechanisms contribute to energy dissipation such as air-damping, squeezed-film damping, acoustic radiation from the supports of the beam (also called anchor or clamping losses), damping due to crystallographic defects (such as dislocations and grain boundaries) and thermoelastic damping [8]. Some of these sources of
energy losses are considered extrinsic such that they can be altered by changing the design or operating conditions. For example, operating the device in vacuum and designing nonintrusive supports reduces air-damping and clamping losses, respectively. However, intrinsic sources of dissipation, such as thermoelastic damping, impose a strict upper limit on the attainable quality factors of a resonator.

II THEORY OF THERMO ELASTIC DAMPING (TED)

Zener predicted that thermoelastic losses may be a limitation to the maximum Q factor of a resonator [9]. Basically, the principle of thermoelastic damping is the following: When a mechanical structure vibrates, there are regions where compressive stress occurs and others where tensile stress occurs, in a cyclic way given by the vibration frequency. Accordingly, compressed regions heat up and stretched regions cool down. Hence a temperature gradient is established between different regions of the system. However, to set the mechanical system in vibration, energy must be provided, leading to a non-equilibrium state having an excess of energy. Disregarding thermoelastic damping, the vibration could persist indefinitely in an elastic body that is perfectly isolated from its environment. However, local temperature gradients lead to irreversible flow of heat, which is a dissipation mechanism that attenuates the vibration until complete rest is achieved. Heat flow through a thermal resistance will result in power dissipation, which is a Q limiting energy loss mechanism. This loss is the most prominent when the period of the resonator is of the same order as the thermal time constant across the beam. From a thermodynamic standpoint TED can be viewed as the initial flexing of the beam which causes the temperature profile of the beam to become more ordered. If the beam re-establishes equilibrium this order is lost, resulting in an irrecoverable increase in entropy, which is an energy loss[10].

A. The concept of the Quality factor

For a one degree of freedom mass–spring system under viscous damping, the equation of motion would be as follows [4]

$$m \ddot{x} + c \dot{x} + kx = 0$$  \hspace{1cm} (1)

$$\ddot{x} + 2\zeta \omega_0 \dot{x} + \omega_0^2 x = 0$$  \hspace{1cm} (2)

$$\zeta = \frac{c}{2\sqrt{km}}\, , \, \omega_0 = \sqrt{\frac{k}{m}}$$  \hspace{1cm} (3)

where $m$ is the mass, $c$ is the viscous coefficient, $x$ is the displacement of mass, $1/(2\zeta)$ is the quality factor of system, for $\zeta<<1$; $\omega_0$ is the natural frequency of the system, and the dot sign shows the differentiation with respect to time. The quality factor of system, $1/(2\zeta)$, depends on the value of mass, viscous coefficient and spring coefficient. The free vibration response of the system may be assumed as the complex form $Xe^{i\omega t}$ where $X$ is the complex amplitude, and $\omega_0$ is the free vibration frequency. Then by substituting $Xe^{i\omega t}$ into the above equation gives

$$\omega^2 - 2\zeta \omega_0 \omega i - \omega_0^2 = 0 \Rightarrow$$

$$\omega = \zeta \omega_0 i \pm \sqrt{1 - \zeta^2 \omega_0^2} \Rightarrow$$

$$\frac{1}{2\zeta} \approx \frac{\text{Re}(\omega)}{2\text{Im}(\omega)} = \text{Qualityfactor}$$  \hspace{1cm} (4)

B. General expressions for TED Factor (Dissipation Factor)

Consider a resonator based on a flexural beam. When the beam bends, one side is in compression and heats up and the other is in tension and cools down. The relaxation time for the heat to travel from the hot side to the cold side depends on the thickness of the beam and on the thermal conductivity of the material. This relaxation time corresponds to a characteristic frequency. When the natural frequency of the resonator becomes comparable to this characteristic frequency maximum dissipation occurs.

Zener’s solution [9] for thermo elastic damping in a thin beam can be approximated as a term Thermoelastic Damping Factor (TED Factor) or Dissipation Factor denoted as $Q^{-1}$ which gives an idea of the internal friction in a resonator. Actually $Q^{-1}$ is the fraction of energy dissipated per radian of vibration and can be expressed as
\[ Q^{-1} = \Delta_E \frac{\omega_0 \tau}{1 + (\omega_0 \tau)^2} \]  
\[ \Delta_E = \frac{E \alpha^2 T_0}{\rho C_p} \]  
where 
\[ \tau = \frac{h^2 \rho C_p}{\pi^4 k} \]  
and \( \omega_0 \) is the undamped natural frequency for the relevant mode [10].

For a simply supported beam, the first natural frequency is
\[ \omega_0^2 = \frac{\pi^4 Eh^2}{12 \rho L^4} \]  
Lifshitz and Roukes’ precise solution can be expressed in the following form [1]
\[ Q^{-1} = \frac{E \alpha^2 T_0}{\rho C_p} \left( \frac{6}{\xi^2} - \frac{6 \sin \xi + \sinh \xi}{\xi^2 \cos \xi + \cosh \xi} \right) \]  
where
\[ \xi = h \sqrt{\frac{\omega_0 \rho C_p}{2k}} \]  

The symbols used in the above equations are:
- \( E \) (Pa)- Young’s modulus, \( \alpha \) -Thermal expansion coefficient, \( k \) (W/m-K)- Thermal conductivity, \( C_p \) (J/kg-K)- Specific heat, \( \rho \) (kg/m³)-Density, \( T \) (K)-Temperature, \( h \) (m)-Thickness and \( L \) (m)-Length

\[ C. \text{ Principles of Modeling of the MEMS Resonator} \]

The modeling approach for the MEMS resonator consists of principles based on descriptions (partial differential equations (PDEs) and functional relations) of relevant effects in three physical domains [11]. These are the mechanical, electrical and the thermal domains. The current approach allows model parameters to be linked to actual physical and geometric parameters.

Thermoelastic damping results from the coupling between the heat equation in the thermal domain and structural dynamics in the mechanical domain through thermoelastic material behaviour. TED is calculated using a complex frequency method in which it is expressed in terms of a complex resonant frequency. This approach uses the eigenvalues and eigenvectors of the uncoupled thermal and mechanical dynamics equations to calculate damping. The numerical implementation of this method has been conducted using finite element solver- COMSOL Multiphysics software-where several partial differential equations are numerically solved with complex frequency values being involved. Using a finite element formulation, a perturbation of the temperature field is explicitly applied to the governing equations associated with heat transfer, thermoelasticity, and structural vibration. This results in an eigenvalue equation with the imaginary part of the eigenvalue representing the frequency of the harmonic vibration and the real part representing the decaying rate of the amplitude [12]. The advantage of the method lies in that it is very easy to extend the same formulation to solve a problem with arbitrary geometry and complicated structures. Also the thermal modes that contribute most to damping can be identified and this information may be used to design devices with higher quality factors.

\[ \text{III. SIMPLE FIXED-FIXED TYPE BEAM RESONATORS} \]

The resonator is a beam of Polysilicon with length 400 μm, height 12 μm, and width 20 μm. The beam is fixed at both ends, and it vibrates in a flexural mode in the z direction (that is, along the smallest dimension). The model assumes that the vibration takes place in vacuum. Thus there is no transfer of heat from the free boundaries. The model also assumes that the contact boundaries are thermally insulated [8].

In order to gain information about the quality of the resonator, its natural frequency and Q value should be known. To find the eigenvalues for the system an eigen frequency analysis is done using COMSOL multiphysics software. For a system with damping, the eigenvalue \( \lambda \) contains information about the natural frequency and Q value [6]. Fig.1 shows the variation of TED factor with eigen frequency for a PolySi based simple beam resonator. From the analysis it is clear that at some particular frequency internal friction (TED factor) is maximum and this corresponds to the maximum dissipation of
the resonator. Maximum energy loss accounts for the minimum Q factor at some particular frequency. From the analysis it is seen that certain thermal modes corresponds to maximum energy dissipation and proper knowledge of this modes can be used for designing resonators with high Q factors.

Fig. 1: TED Factor versus Eigen Frequency of a Simple fixed-fixed PolySi beam resonator.

Q factor of a simple fixed-fixed type resonator is highly material dependent. It depends on the parameters such as Young’s Modulus (E), Thermal expansion Coefficient (\( \alpha \)), Density of the material (\( \rho \)) and Poisson’s ratio (\( \nu \)). The variation of Q factor with and without thermoelastic damping (TED) is summarized in Table I.

Table I: shows the variation of Q factor (with and without TED effect) with materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>E (GPa)</th>
<th>( \alpha )</th>
<th>( \rho ) (kg/m³)</th>
<th>( \nu )</th>
<th>Eigen Freq</th>
<th>Q without TED</th>
<th>Q with TED</th>
</tr>
</thead>
<tbody>
<tr>
<td>PolySi</td>
<td>160E9</td>
<td>2.4E-6</td>
<td>2320</td>
<td>0.22</td>
<td>6.9E5</td>
<td>2.104E11</td>
<td>9492.73</td>
</tr>
<tr>
<td>GaAs</td>
<td>85.9E9</td>
<td>5.7E-6</td>
<td>5316</td>
<td>0.31</td>
<td>8.49E5</td>
<td>1.2102E12</td>
<td>6600.925</td>
</tr>
<tr>
<td>ZnO</td>
<td>210E9</td>
<td>5.5E-6</td>
<td>5676</td>
<td>0.33</td>
<td>4.70E5</td>
<td>1.126E12</td>
<td>6806.72</td>
</tr>
<tr>
<td>Si₃N₄</td>
<td>250E9</td>
<td>2.3E-6</td>
<td>3100</td>
<td>0.23</td>
<td>6.91E5</td>
<td>8.892E11</td>
<td>7770.43</td>
</tr>
<tr>
<td>Al</td>
<td>70E9</td>
<td>23.1E-6</td>
<td>2700</td>
<td>0.35</td>
<td>3.99E5</td>
<td>3.60E11</td>
<td>270.16</td>
</tr>
<tr>
<td>Cu</td>
<td>120E9</td>
<td>1.0E-6</td>
<td>8960</td>
<td>0.34</td>
<td>7.75E5</td>
<td>2.44E12</td>
<td>292.892</td>
</tr>
</tbody>
</table>

In this paper, effect of material properties of the resonator beam on the Q factor with and without thermoelastic damping (TED) is analyzed. When semiconductors are considered it is seen that compared to GaAs, PolySi provides better Q value and less thermoelastic damping. The analysis of ZnO and Si₃N₄, which are the commonly used insulators, shows that Q factor with TED effect (\( Q_{TED} \)) is highly reduced. The performance of metals such as Al and Cu are analyzed in terms of Q factors with and without TED effect and shows that reduction in Q with TED (\( Q_{TED} \)) is very large as compared to that of semiconductors and insulators. In terms of Q factor with TED the performance of metal based resonators will be worse than semiconductors and insulators. Without TED effect all type of materials give high Q value as given in the Table I. Most commonly semiconductors are the preferred material for MEMS resonators.

Fig. 2 shows the analysis of a simple PolySi based fixed-fixed beam resonator in terms of Q factor and varying geometry. The changes in the dimensions of the resonator highly affects its Q factor. In this paper, Q factor with TED effect (\( Q_{TED} \)) is analyzed for different lengths of the beam with width and height kept as constants.

It is seen that at some particular length there is a huge transition for Q value and it is proposed that this length is the critical length of the resonator. In this paper, the critical length of the resonator corresponds to a value of 280µm. Above this length Q factor suddenly increases and eigen frequency values becomes high. When the minimum length of the beam of the resonator is below 280 µm, eigen frequencies are very small and Q factor also drops to a low value. We propose that while designing a resonator with high Q value this critical size should be essentially considered.

Fig. 2: Q factor versus Length of a Poly Si based simple fixed-fixed beam resonator.

Fig. 3 and Fig. 4 show the simulated outputs of a simple fixed-fixed Poly Si beam resonator for the first eigen mode which corresponds to an eigen frequency of 633.9414KHz. The size of the resonator is above the critical length i.e. L > 280 µm. The colour variation for different variables in
the plots corresponds to the colour chart at the right side showing the maximum and minimum.

Fig.5 and Fig.6 show the simulated outputs of a simple fixed-fixed PolySi beam resonator at length less than the critical length of the resonator i.e.L<280 µm. The first eigen mode corresponds to a very low eigen frequency of 1.044E−8Hz. This reduction in eigen frequency accounts for the sudden fall in Q value of the resonator. The total displacement of the resonator is also a very small value. As in the previous case the colour variation for different variables in the plots indicates the colour profile at the right side in accordance with the maximum and minimum.

In this paper, the effect of geometry variation is analyzed in the case of a simple PolySi based fixed-fixed type resonator. Simulated outputs are obtained for different lengths with width and height kept as constants. In this analysis all simulations are done with Width=20 µm and Height=1.2 µm.

Fig.3: Simulated TED output of a simple fixed-fixed PolySi beam resonator showing total displacement (Max=27.11 µm and mini=0) for L=282 µm; Width=20 µm and Height=1.2 µm.

Fig.4: Simulated TED output of a simple fixed-fixed PolySi beam resonator showing temperature distribution (Max =2.842 and mini=-2.821) for L=282 µm; Width=20 µm and Height=1.2 µm.

Fig.5: Simulated TED output of a simple fixed-fixed PolySi beam resonator showing total displacement (Max=0.03922 nm and mini=0) for L=278 µm; Width=20 µm and Height=1.2 µm.

Fig.6: Simulated TED output of a simple fixed-fixed PolySi beam resonator showing temperature distribution (Max=1.732 and mini=-1.732) for L=278 µm; Width=20 µm and Height=1.2 µm.

IV. THIN FILM RESONATOR WITH STRAIGHT AND FOLDED CANTILEVERS

Almost all surface-micromachined thin films are subjected to thermal stress, which accompanies a change in temperature. For a lateral resonator with four cantilever-beam springs, the resonant frequency is [14]

\[
fo = \frac{1}{2\pi} \sqrt{\frac{4Etb^3}{mL^3} + \frac{24\sigma_t tb}{5mL}}
\]

(11)

where \(m\) is the mass of the resonator plate, \(E\) is Young’s modulus, \(t\) is the thickness, \(L\) is the length, \(b\) is the width, and \(\sigma_r\) is the residual stress in the cantilevers. The stress is typically a sum of external stresses, the thermal stress, and intrinsic components. Assuming the material is isotropic, the
stress is constant through the film thickness, and the stress component in the direction normal to the substrate is zero.

The laws of thermodynamics predict that a variation of strain in a solid is accompanied by a variation of temperature, which causes an irreversible flow of heat. This heat conduction further gives rise to an increase in entropy and consequently to dissipation of vibration energy termed as thermoelastic damping. [9]. For a thin film resonator with four straight cantilever-beam springs, when subjected to thermal stress, strain gradients are generated which in turn leads to temperature gradients and irreversible flow of heat, causing internal energy dissipation. Thermoelastic damping, which is the internal energy dissipation mechanism increases the eigen frequency and degrades the Q factor of the resonator [13].

In this work, it is observed that TED factor increases with increase in eigen frequency and so it can be predicted that internal friction or dissipation increases with eigen frequency. This increase in internal energy losses degrades the Q factor at higher eigen frequencies as shown in Table III.

Fig.7 to Fig.9 show the simulated outputs for a thin film resonator with straight cantilevers indicating the distribution of temperature along the surface of the resonator with increasing eigen frequencies. The variation of total displacement along the boundary is also shown in these figures. The colour variation across the surface of the thin film resonator exhibits the corresponding temperature variation as provided in the colour chart at the right side of the plot. The temperature profile is different for different eigen frequencies as shown in these figures.

The flexures relieve axial stress because each is free to expand or contract in the axial direction and sensitivity to stress is thus reduced. The first and last springs are cantilever beams. The spring constant for them can be obtained from $k = \frac{3EI}{L^3}$, where $I$ is the moment of inertia.
For a rectangular beam with a rotation about the y-axis, the moment of inertia is \( I = w^2t/12 \), where \( w \) is the width and \( t \) is the structure’s thickness. The second spring can be taken as a column with a spring constant of \( k = AE/L \), where \( A \) is the cross-sectional area \( A = wt \). Assuming the spring thickness and width are the same everywhere, the equation comes to [14]

\[
L_{eq}^3 = L_1^3 + \frac{w^2L}{4} + L_3^3
\]

(12)

which can help estimate the lengths of the folded springs.

The basic folded structure is a U-shaped spring. For springs in series the equivalent spring constant is [14]

\[
\frac{1}{k_{eq}} = \frac{1}{k_1} + \frac{1}{k_2} + \frac{1}{k_3}
\]

(13)

In this work, it is observed that like in the case of a thin film resonator with straight cantilevers, TED factor increases with increase in eigen frequency. It can be predicted that internal friction or dissipation increases with eigen frequency but its value gets reduced as compared to that of a TFR with straight structure. As the TED Factor decreases, Q factor improves. The improvement in the Q factor and reduction in the eigen frequencies are the main advantages of the proposed folded structure compared to the straight structure. The improvement in Q factor for a thin film resonator (TFR) with folded cantilever structure when compared to a thin film resonator with straight cantilever is due to this increase in eigen frequency.

Table III: Comparison of Q_{withoutTED} and Q_{withTED} values for a Thin Film Resonator (TFR) with straight and folded cantilevers.

<table>
<thead>
<tr>
<th>TFR-straight</th>
<th>TFR-Folded</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q_{withoutTED}</td>
<td>Q_{withTED}</td>
</tr>
<tr>
<td>Q_{withoutTED}</td>
<td>Q_{withTED}</td>
</tr>
<tr>
<td>8.0812E11</td>
<td>11746.52</td>
</tr>
<tr>
<td>2.0400E11</td>
<td>11697.97</td>
</tr>
<tr>
<td>1.6286E10</td>
<td>11676.66</td>
</tr>
<tr>
<td>5.2447E10</td>
<td>4255.32</td>
</tr>
<tr>
<td>6.9305E10</td>
<td>4255.23</td>
</tr>
<tr>
<td>4.5552E10</td>
<td>4248.69</td>
</tr>
<tr>
<td>8.3342E10</td>
<td>4248.72</td>
</tr>
</tbody>
</table>

The eigen frequencies for the next higher modes are also reduced to 4.926KHz and 18.864KHz for the folded structure. But for a thin film resonator with straight cantilevers after the first mode, the next higher modes corresponds to frequencies of 417.92KHz and 458.1313KHz. In this paper, we propose that the increase in the internal dissipation and simultaneous decrease in Q factor for a thin film resonator with straight cantilever is due to this increase in eigen frequency.

Fig. 9: Simulated output of a Thin Film Resonator with folded cantilevers showing temperature distribution and displacement for Eigen frequency=957.716Hz.

Fig.10: Simulated output of a Thin Film Resonator with folded cantilevers showing temperature distribution displacement for Eigen frequency=4.926KHz.
Fig. 11: Simulated output of a Thin Film Resonator with folded cantilevers showing temperature distribution and displacement for Eigen frequency=18.864KHz.

V. ACKNOWLEDGMENT
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VI. CONCLUSION
This paper shows the importance of Thermoelastic damping (TED) as an energy loss mechanism in MEMS based resonators. TED effects on RF MEMS resonators such as simple fixed-fixed PolySi beam resonator and thin film resonators with straight and folded structures are analyzed using COMSOL Multiphysics software. The effect of material properties and geometry on TED characteristics is studied in the case of a simple fixed-fixed type resonator. In order to get a reasonable Q value with TED effect (Q_{TED}), the critical size of the beam is essential for geometry. By proper identification of the thermal modes that contribute most to damping resonators with high quality factors can be developed. In the case of thin film resonators a new geometry is developed to reduce TED effects. By attaching folded springs to the existing MEMS structures, the effect of temperature on eigen frequency and Q factor can be reduced to a certain extent. The folded springs relieve axial stress because it is free to expand or contract in the axial direction and so sensitivity to stress can be reduced. Q factor is improved with this added geometry. Increasing the Q factor improves the signal-to-noise ratio (SNR), spectral purity, and selectivity of the system. It is therefore important to be able to predict the Q factor of a structure and have accurate design guidelines to minimize the energy losses.

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