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INVESTIGATION OF THERMOELASTIC LOSS MECHANISM IN SHELL RESONATORS

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ABSTRACT

Maximizing quality (Q) factor is key to enhancing the performance of micro mechanical resonators, which are used in a wide range of applications such as gyroscopes, filters, and clocks. There are several energy loss mechanisms commonly associated with micro resonators including anchor loss through the substrate, squeeze film damping, thermoelastic dissipation (TED), and surface loss. This work focuses on the thermoelastic loss as one of the major energy dissipation mechanisms of micro shell resonators.

In this article, the effects of material properties, thickness, conductive coating and operating temperature on the Q -factor of micro shell resonators are investigated. Numerical simulation shows shell resonators have higher Q -factors when they are operating at lower temperatures. Although, the magnitude of the simulated Q -factors of an uncoated bare resonator made from fused silica is more than 70 million and so it is too high to have a remarkable effect on the total Q -factor, our study shows that even a thin layer of some conductive coatings like gold on the surface of a bare shell reduces Q -factor significantly. The sensitivity of the coated shell resonator design to the TED phenomenon provides useful information for the development of new micro shell resonators with improved performance and Q -factors.

Keywords: Thermoelastic Dissipation, Quality Factor, Shell Resonators, Conductive Coating, Gyroscope.

INTRODUCTION

Micro electro mechanical systems (MEMS) are being developed for a wide range of applications [1]. Low manufacturing cost, high durability, low weight, small size, low energy consumption, and capability of incorporating more complex functions make them highly attractive [2, 3]. Successful microstructures rely not only on well-developed fabrication technologies, but

also on the device design and knowledge of device behavior [4, 5]. One of the most important MEMS is the mechanical resonators. In order to achieve high performance, a resonator must have low energy dissipation and a very high Q -factor. Recently, micro shell structures were introduced as low-cost resonators with potential for batch fabrication processing [6].

Several different phenomena can lead to energy dissipation in micro shell resonators. When they resonate, some of their vibrational energy is dissipated due to wave propagation into the anchor of the resonator. This phenomenon is called anchor loss. In order to reduce anchor loss, resonators should be designed with their anchor at the nodal point of the mechanical wave to prevent propagation of elastic waves to the support media. Surface loss is another energy dissipation mechanism in the resonators, especially when their size is small such that their surface-to-volume ratio is large [7]. Squeeze film damping — the result of movement of trapped gas into and out of the space between moving and stationary parts of a resonator, which is opposed by the gas viscosity can also be a major energy loss mechanism in resonators [8]. This phenomenon produces a pressure distribution on the resonator surface that acts as a damping force [9]. In order to reduce it, most resonators are operated in very low gas pressure environments (less than a Torr) that do not cause loss due to squeeze film damping.

In resonant systems, some regions of the structure experience tension while others experience compression in a cyclic pattern. Tensile and compressive stresses produce cold and hot regions in the resonator and so there are periodic local temperature gradients in the structure. In order to relax back to equilibrium, energy dissipates through irreversible heat flow and entropy generation in the resonator, a process known as thermoelastic dissipation (TED) [10, 11]. If any of the

thermal transport time constants of the resonator are close to the deflection period of elastic deformation of the structure, Q_{TED} of the system is reduced and the resonator suffers significant energy loss [12].

In the 1930s, Zener [13, 14] presented a general model for calculating the thermoelastic Q -factor of wires and reeds by considering one-dimensional heat transfer across the bending direction. Nayfeh and Younis [15] analytically modeled Q_{TED} of micro plates with general shapes and boundary conditions. They showed that the geometric properties of a microplate could have a significant effect on the Q -factor. The effect of temperature on the Q -factor of double-ended tuning fork resonators due to thermoelastic dissipation was simulated by Ghaffari et al. [16]. Chandler et al. [17] studied the effect of slots between the hot and cold regions of microbeam resonators on Q_{TED} both theoretically and experimentally. Ghaffari and Kenny [11] analyzed the effect of a silicon dioxide thin film on thermoelastic dissipation in silicon micro resonators. They showed that a thin film affects thermal relaxation of the resonator and changes its Q -factor. Recently Cho et al. [6, 18] fabricated three-dimensional (3D) shell resonators made out of fused silica. They showed that when this shell vibrates in the wineglass modes it can be used as a MEMS gyroscope. In order to achieve high sensitivity and low energy consumption, shell gyroscopes need to have a high Q -factor, so understanding energy loss mechanisms is extremely important for the improvement of shell gyroscopes.

This paper studies the Q -factor of shell resonators due to thermoelastic damping. The relationships between Q -factor and material properties of a resonator such as thermal expansion coefficient and thermal conductivity are explored. Effects of conductive coatings on the surface of a resonator are investigated. It is shown that even a thin film coating can significantly reduce the Q -factor. The effect of operation temperature on energy dissipation within a shell resonator is analyzed numerically and it is shown that shell resonators have a lower Q -factor at elevated temperatures.

PROBLEM CHARACTERIZATION

In thermoelastic mechanics, the elastic field is coupled to the thermal field. Three-dimensional elastic equations of motion can be written as:

$$\frac{E}{2(1+\nu)} \nabla^2 \mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)} \nabla(\nabla \cdot \mathbf{u}) - \frac{E\alpha}{3(1-2\nu)} \nabla T + f = \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} \quad (1)$$

where E , ν , α , ρ are Young's modulus, Poisson's ratio, coefficient of thermal expansion, and density of the material respectively, f is the external force per volume, $\mathbf{u}=(u, v, w)$ is the deformation vector, and T is temperature. The thermal dynamics governed by the heat conduction equation

$$k \nabla^2 T - \rho C_{sp} \frac{\partial T}{\partial t} = \frac{E\alpha T}{1-2\nu} \frac{\partial}{\partial t} \nabla \cdot \mathbf{u} \quad (2)$$

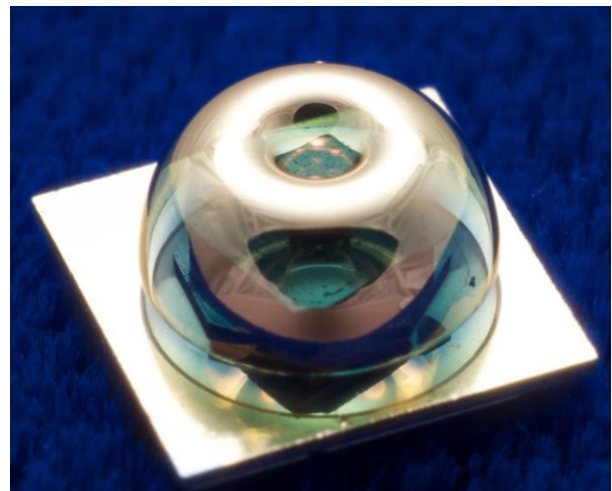
where k is thermal conductivity, and C_{sp} is specific heat capacity of material. In most cases, T in the right-hand side of Eq. (2) can be replaced by nominal average temperature T_0 to yield a linear equation for the temperature [14]. These two equations could be solved using a finite element-based approach for arbitrary 3D geometries to find deformations and temperature. In the resonators, the ratio of stored vibrational energy to energy dissipated per vibration period is defined as Q -factor and it can be found from Eq. (3) [9].

$$Q_i = \frac{1}{2} \left| \frac{\text{Re}(\omega_i)}{\text{Im}(\omega_i)} \right| \quad (3)$$

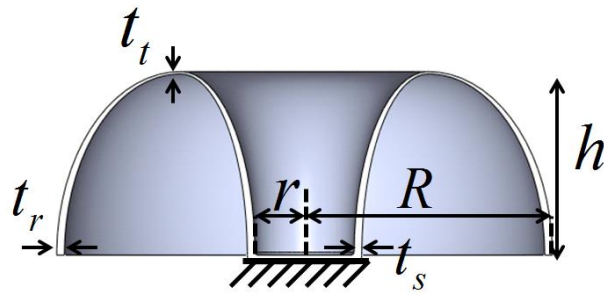
where Q_i is Q -factor and ω_i is resonant frequency of i 'th mode. COMSOL Multiphysics is used to solve fully coupled thermo-mechanical finite element eigenfrequency problem to obtain Q_{TED} numerically.

Fused Silica Micro Birdbath

The shell resonator shown in Fig. 1 is considered for simulations. It has the shape of semi-toroid or birdbath, and it is called the birdbath resonator. It has an axisymmetric shape with varying thickness along its curvature such that the top part of the structure has the thinnest cross section (Fig. 1(b)). To fabricate this structure, a thin fused silica substrate is placed on top of a mold and a torch with temperature higher than 1600° C is approached to the surface of the wafer. At this temperature, the substrate starts to reflow following the shape of the graphite mold. The shell is released from the flat substrate using lapping and chemical-mechanical polishing (CMP) processes. The shell has sub-nanometer surface roughness. The shell is then bonded to a bottom silicon substrate using glass frit or Crystalbond 509 (SPI Supplies, West Chester, PA, USA) [6]. The most important geometric parameters of the shell are illustrated in Fig. 1(b). They include radius R , top part thickness t_t , rim thickness t_r , support thickness t_s , support radius r , and shell height h .



(a)



(b)
Fig. 1. (a) Fused silica birdbath resonator photograph.
 (b) Cross sectional view of a shell resonator [6].

A modal analysis is conducted to calculate the fundamental frequencies and mode shapes of the shell. The first five resonance modes of this shell are shown in Fig. 2.

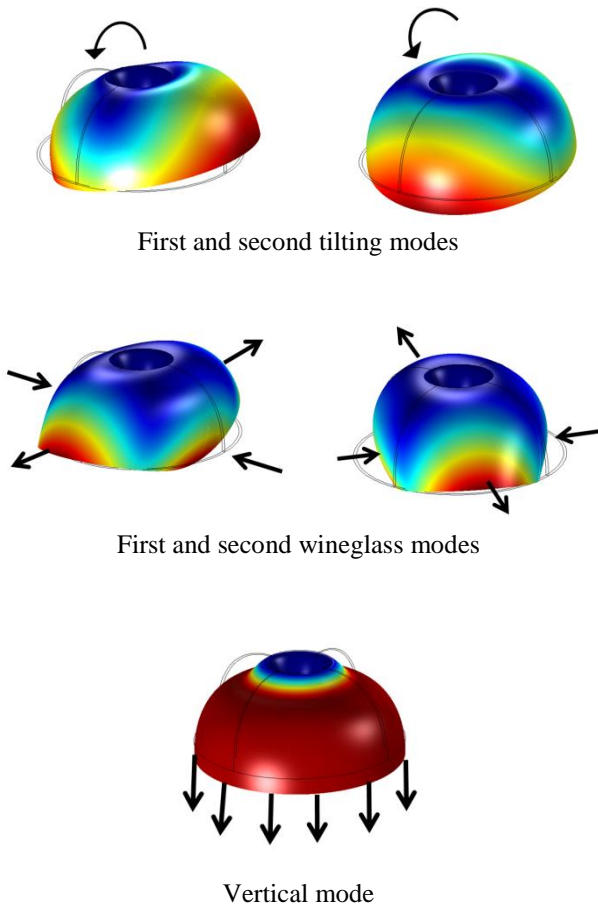


Fig. 2. First five modes of the shell resonator.

A shell resonator operating in the wineglass modes can be used as a gyroscope. To achieve high gyroscopic performance, the shell resonator needs to have low energy dissipation and a very high Q -factor in these modes. In order to simulate Q_{TED} , a shell with the mesh configuration shown in Fig.3 is considered. The properties used in the simulation given in Table 1.

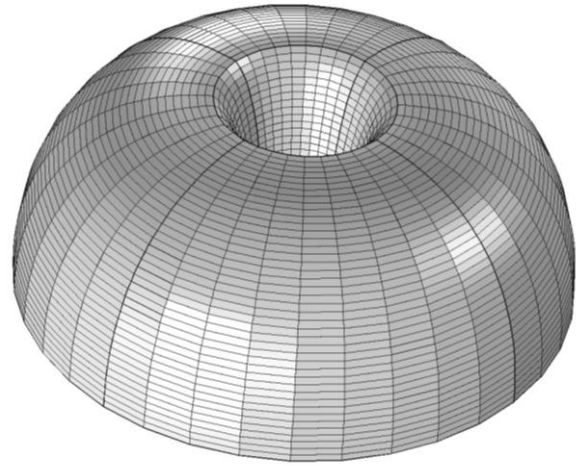


Fig. 3. Meshed configuration of a shell structure with characteristics given in Table 1.

Table 1. Geometric properties of simulated shell.	
Parameter	Value
R_o	2500 μm
r_o	400 μm
t_o	30 μm
t_{ro}	70 μm
t_{so}	100 μm
h_o	1900 μm

RESULTS AND DISCUSSION

Fused silica is chosen as the reference material, with Young's modulus $E_{FS} = 70$ GPa, Poisson's ratio $\nu_{FS} = 0.17$, density $\rho_{FS} = 2200$ kg/m³, thermal conductivity $k_{FS} = 1.4$ W/(m.K), specific heat capacity $C_{sp_{FS}} = 730$ J/(kg \times K), and coefficient of thermal expansion $\alpha_{FS} = 5 \times 10^{-7}$ 1/K.

By solving equations (1) and (2) numerically at $T_o = 293.15$ K for the structure shown in Fig. 3, the eigenvector that includes deformation and temperature in each node, and the corresponding eigenvalue are calculated. The simulated temperature distribution of a deformed shell is shown in Fig. 4. Large temperature gradients are found at the rim and the top part of the shell. These regions are responsible for large TED. These are the regions with a large stress concentration and a large shell curvature. By using results of the eigenvalue simulation and Eq. (3), the thermoelastic Q -factor of the fused silica shell is found to be 76.5 million.

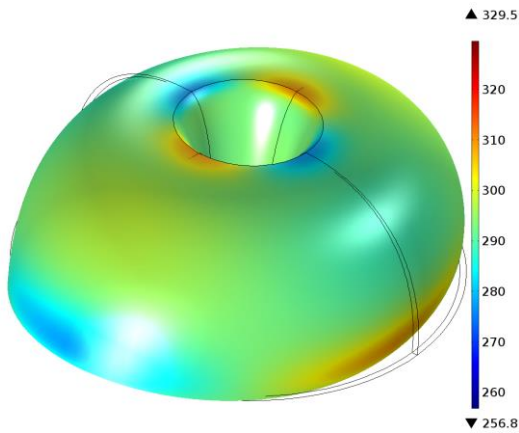


Fig. 4. Temperature distribution of a shell resonator in wineglass mode.

Effect of Material Properties

As shown in equations (1) and (2), the thermo-mechanical behavior of resonators depends on Young's modulus, specific heat capacity, density, Poisson's ratio, coefficient of thermal expansion, and thermal conductivity. In order to compare the effect of different material properties, one property is changed while the others are fixed at their intrinsic values for fused silica. Fig. 5 shows the variation in the normalized thermoelastic Q -factor, which is defined as Q/Q_{FS} versus the change of normalized material properties.

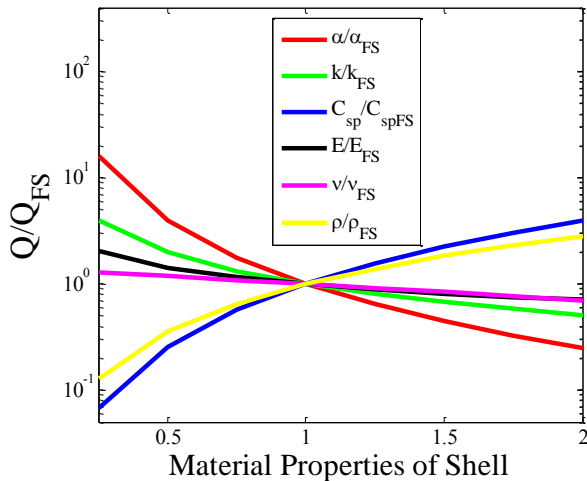


Fig. 5. Effect of material properties on the normalized Q -factor of shell resonators.

As shown in this figure, the Q -factor of these resonators decreases as α increases. The physical expansion caused when temperature changes, produces thermal stress. The entropy of the resonator during expansion is a function of α , so by increasing α irreversible energy flow between elastic and thermal domains increases and Q_{TED} decreases. In fact, the thermal expansion coefficient is a parameter that couples the thermal and mechanical domains together. Fig. 5 shows that reducing thermal conductivity can also enhance Q -factor because it reduces heat transfer from hot to cold regions. In equations (1) and (2), all the terms with α as a coefficient also include E , so

increasing Young's modulus will amplify the coupling between the mechanical and thermal domains leading to a lower Q -factor. By increasing density and specific heat capacity, the heat capacity of the material $C = \rho C_{sp}$ increases, which helps reduce irreversible heat transfer that can improve Q -factor as shown in Fig. 5. Indeed, thermal diffusivity $k/(\rho C_{sp})$ can affect Q -factor remarkably, implying that it is essential to select materials with low thermal diffusivity in order to improve Q -factor.

Effect of Thickness

In this section, the effect of thickness of a shell's structure on Q -factor is analyzed by changing the thickness of different parts. First, the thickness of the shell rim is changed as shown in Fig. 6.

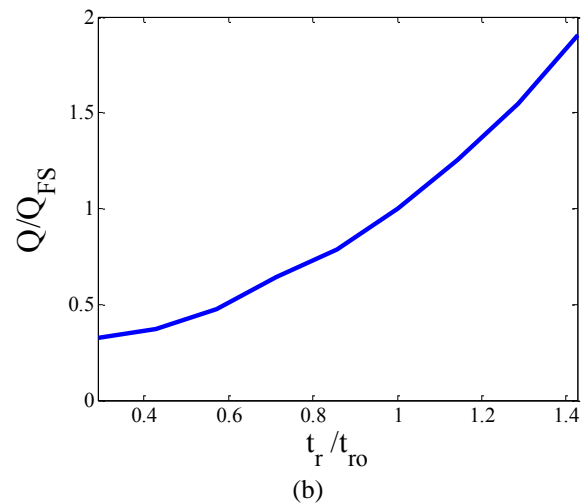
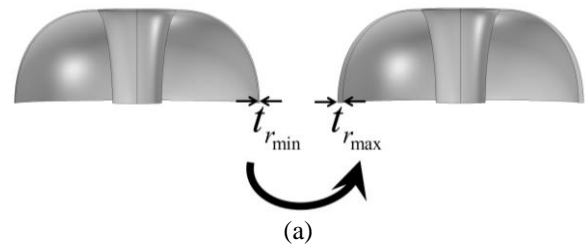
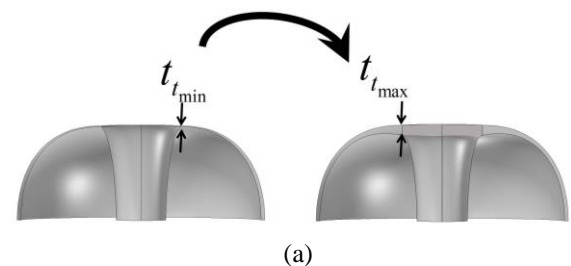


Fig. 6. (a) Changing thickness of rim. (b) Normalized Q -factor versus normalized rim thickness.

Numerical simulation shows that increasing the thickness of the rim can reduce thermoelastic dissipation of the resonator, so in order to have a high Q -factor, the resonator rim should be as thick as design constraints allow.

Second, the effect of thickness of the top part of the shell on the Q -factor is analyzed, as shown in Fig. 7.



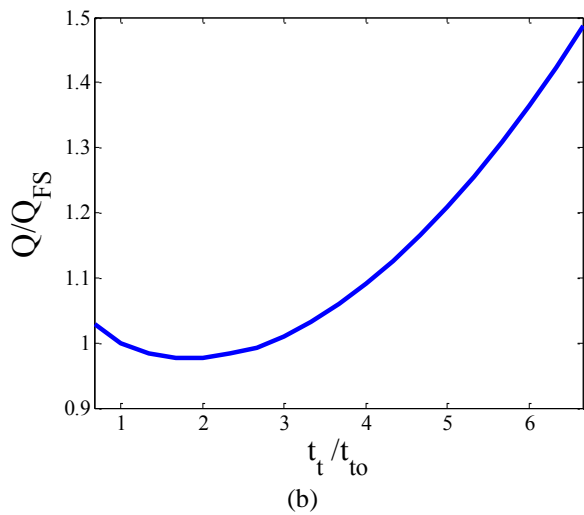


Fig. 7. (a) Changing thickness of top. (b) Normalized Q -factor versus normalized thickness of top.

The thickness is changed from $20\ \mu\text{m}$ to $200\ \mu\text{m}$ and the normalized Q -factor is plotted versus normalized thickness in Fig. 7. The numerical results shows that to achieve a high Q -factor, the thickness of the top part should be much larger than $60\ \mu\text{m}$.

Effect of Ambient Temperature

Eq. (2) shows that the coupling term between the thermal and mechanical domains is a function of temperature. According to this equation, coupling increases as temperature increases. In order to investigate the effect of temperature, the working temperature of the resonator is changed and Q -factor is calculated for the new equilibrium condition. In this simulation, the material properties of fused silica remain constant while the equilibrium temperature is changed. Fig. 8 shows that the Q -factor reduces as ambient temperature increases.

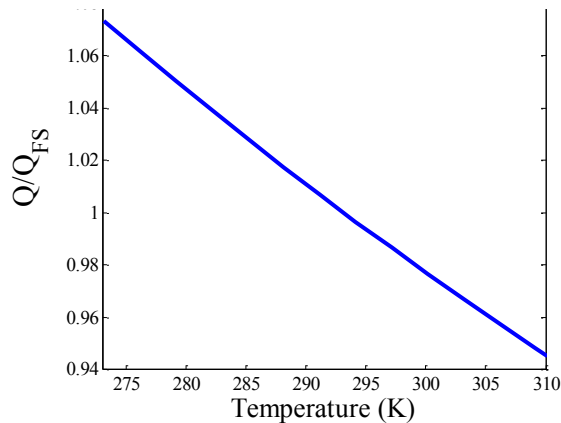


Fig. 8. Normalized Q -factor versus temperature.

Effect of Coating Layer

As discussed in previous sections, in order to have a high Q -factor resonator, it is important that the resonator have low thermal diffusivity and thermal expansion coefficient. Fused silica has a very low thermal conductivity and thermal expansion coefficient and is an excellent candidate for high Q -factor resonators, but its electrical conductivity is also very

low. In order to actuate the resonator by electrostatic force, it is necessary to coat the fused silica shell with an electrically conductive material such as gold, as shown in Fig. 9. Unfortunately, most of the conductive materials have high thermal diffusivity and thermal expansion coefficients, which increase thermoelastic dissipation. Gold, with Young's modulus $E_{Au} = 70\ \text{GPa}$, Poisson's ratio $\nu_{Au} = 0.44$, density $\rho_{Au} = 19300\ \text{kg/m}^3$, thermal conductivity $k_{Au} = 317\ \text{W/(m.K)}$, specific heat capacity $C_{spAu} = 129\ \text{J/(kg}\times\text{K)}$, and coefficient of thermal expansion $\alpha_{Au} = 14.2\times 10^{-6}\ \text{1/K}$ is considered as a conductive coating.

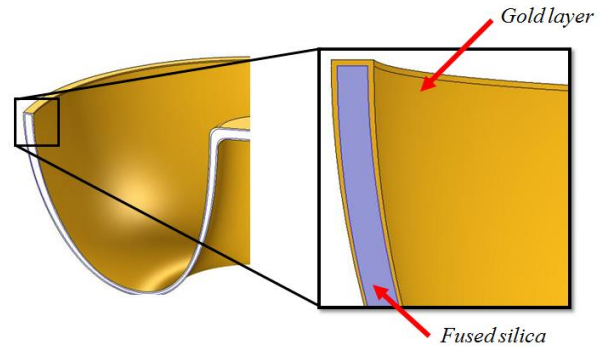


Fig. 9. Shell coated with gold.

The simulation shows that a $1\ \mu\text{m}$ -thick gold layer can increase thermoelastic dissipation of the resonator more than 70 times. The gold layer can be treated as a parallel thermal resistance with low thermal resistivity, causing heat transfer in the shell to increase. It further increases energy dissipation due to its high thermal expansion coefficient, which increases entropy generation in the system. The effect of the gold coating thickness on the normalized Q -factor is shown in Fig. 10. As depicted, even a very thin layer of gold, only $100\ \text{nm}$ thick, reduces the Q -factor of the shell resonator more than 80 %.

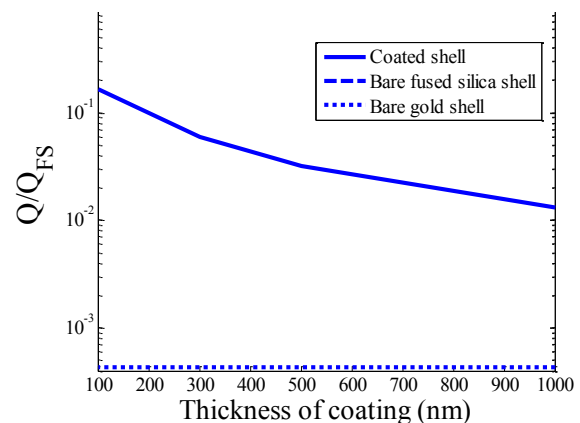


Fig. 10. Normalized Q -factor versus thickness of metal coating.

CONCLUSION

This paper investigates the effect of thermoelastic dissipation on the Q -factor of shell resonators operating in the wineglass mode. It is shown that the material properties have a remarkable effect on the Q -factor of

the shell resonators. It is observed that fused silica with its low thermal diffusivity and thermal expansion coefficient is a promising material for high Q -factor resonators. The effect of the conductive coating on the Q -factor of shell resonators is significant. In fact, a thin gold film reduces thermal resistance between hot and cold regions of the resonator and increases coupling between the thermal and mechanical domains in the system. The effect of thickness f different parts of shell on Q -factor is investigated and optimum design shape for high Q -factor shell resonators is found. It is also shown that as temperature increases, the Q -factor reduces.

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