Thermoelastic damping in layered micromechanical resonators

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SUMMARY. The effect of coatings and superficial oxide on the behavior of micro resonators deserves attention in view of its impact on real-life devices. To this purpose, in this work we focus on the thermoelastic damping in layered thin resonating beams. Including the effect of thermally imperfect interfaces, the quality factor is analytically computed. The results obtained are discussed and compared with available data.

1 INTRODUCTION

In microelectromechanical systems (MEMS) with vibrating parts, such as high-frequency resonators, a critical requirement is often to obtain a low structural damping. If damping is not excessive, the fraction of energy lost per radian can be quantified by the inverse of the so called *quality factor Q*. While strong miniaturization allows the designers to increase the resonant frequency and thus the sensitivity of the resonators, it is difficult to increase the quality factor, as evidenced by several experimental studies [1]. Some sources of extrinsic dissipation can be controlled: for instance, if the devices are packed in a near-vacuum environment, fluid damping becomes negligible, but intrinsic loss mechanisms in the solid limit the quality factor.

Solid or intrinsic damping is induced by a lot of physical and chemical processes, each mechanism is connected to an amount of dissipated energy and, consequently, to a value Q_j. The overall quality factor can therefore be expressed as: $Q = (\sum 1/Q_j)^{-1}$. The thermoelastic damping Ψ is defined as the ratio of the energy dissipated per cycle to the stored elastic energy and is connected to the quality factor by a simple relation:

$$\Psi = \frac{2\pi}{Q} \tag{1}$$

Thermoelastic loss is considered as a fundamental dissipation mechanism in micro-beam bending resonators. This mechanism gives an upper bound of the quality factor which can be evaluated by means of simplified formulae, such as the well-known Zener's expression [2].

The Q factor predicted by a thermoelastic analysis is in good agreement with the quality factor experimentally measured on several silicon single-crystal micro-resonators [3]. On the contrary, the classical thermoelastic analysis is unable to interpret the size effect recently evidenced in resonators when the dimensions become very small, below several microns [1,4]. In [5] the Authors proposed a nonlocal thermoelastic model which can better interpret the observed behavior in a certain range of resonator dimensions. However, for sub-micron and nano-resonators, several causes of additional dissipation, not yet exhaustively investigated, come into play. Intrinsic dissipation of thin coating films and surface loss may become relevant at very small scales, as discussed in [4].

In this work we focus on the effect of the presence of superficial layers, with different thermo-mechanical properties, on the quality factor of micro-beams. At difference with previous works on this subject [6, 7], we include thermally imperfect interfaces between layers: this means that a temperature jump is involved at the interface, with consequences on the thermal behavior of the beam and on the overall dissipation. The quality factor is computed through the procedure that was originally proposed by Zener [2] with reference to homogeneous beams. The thermal field is evaluated by adopting an expansion in series of spatial eigenfunctions [7]. The effect of thermal jump at the interface is introduced as a suitable boundary condition in the eigenvalue problem. The achieved results, with reference to different materials in the thin films, are critically compared with experimental measurement [8]. A parametric study is performed on the effect of imperfect interface, which is tuned by a scalar factor. A strongly non-monotonic behavior of the dissipation level is evidenced and, at least for some material couples, a peak of thermoelastic damping is observed.

2 THERMOELASTIC PROBLEM IN LAYERED BEAMS

2.1 *Problem formulation*

In thermoelastic solids the coupling of the strain field to the temperature field induces the irreversible flow of heat driven by temperature gradient. This process of energy dissipation is called thermoelastic damping (TED) and sets an upper limit to the quality factor of resonators.

In the special case of a thin homogeneous vibrating beam thermoelastic damping can be computed using Zener's approach [2]. In this work we follow a similar analytical approach to calculate thermoelastic dissipation in thin layered beams, schematically shown in Figure 1. Each layer i ($i = 1,\ldots, N$) of thickness h_i is endowed with different elastic and thermal properties (E_i = Young modulus, α_i = thermal expansion coefficient, κ_i = thermal conductivity, C_i = specific heat, ρ_i = density). The following assumptions are made.

- The cross section remains straight and orthogonal to the beam axis (Bernoulli-Euler kinematic hypothesis)
- The heat conduction is limited to the transverse direction
- The interfaces between the layers are not thermally perfect: they can dissipate heat by convection according to Newton's law of cooling (i.e. heat transfer is proportional to the temperature difference between the layers).

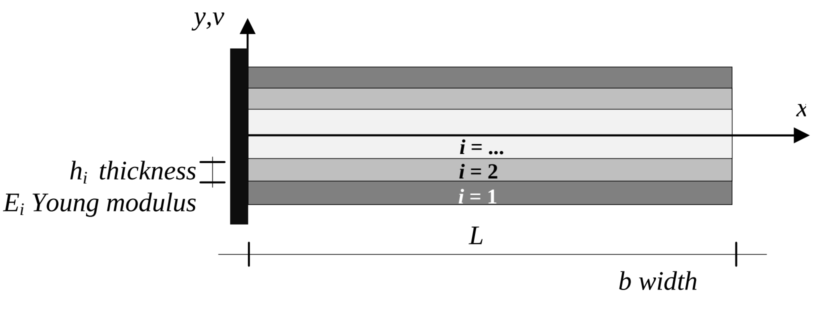

Figure 1: Schematic representation of the layered beam's geometry

According to the Bernoulli-Euler hypothesis axial strain is expressed in terms of the beam's curvature by:

$$\varepsilon = -\frac{d^2 v}{dx^2} y \tag{2}$$

where v is the transversal displacement of the points on the neutral axis. The latter is a horizontal line which passes through the centroid of the homogenized cross-section, identified by the following condition:

$$b\sum_{i=1}^{N}\left[E_i \int_{y_i}^{y_{i+1}} y dy\right] = 0 \tag{3}$$

Stress σ in each layer is expressed by the thermoelastic model, where $\Delta T_i = T_i - T_{0i}$ is the temperature variation with respect to the reference value T_{0i}:

$$\sigma_i = E_i(\varepsilon - \alpha_i \Delta T_i) \tag{4}$$

The bending moment can be computed as follows

$$M = -b\sum_{i=1}^{N}\left[-E_i \int_{y_i}^{y_{i+1}} y^2 dy \frac{d^2 v}{dx^2} - E_i \alpha_i \int_{y_i}^{y_{i+1}} \Delta T_i y \; dy\right] \tag{5}$$

and the dynamic equilibrium equation for free vibrations reads

$$\sum_{i=1}^{N} \rho_i h_i \ddot{v} - \frac{d^2}{dx^2}\sum_{i=1}^{N}\left[-E_i \int_{y_i}^{y_{i+1}} y^2 dy \frac{d^2 v}{dx^2} - E_i \alpha_i \int_{y_i}^{y_{i+1}} \Delta T_i y \; dy\right] = 0 \tag{6}$$

If one neglects heat conduction along the longitudinal direction of the beam, the heat equation in each layer is:

$$\dot{T}_i = \beta_i \frac{d^2 \dot{v}}{dx^2} y + \lambda_i \frac{\partial^2 T_i}{\partial y^2} \qquad y_i < y < y_{i+1} \qquad i = 1,...N \tag{7}$$

where $\beta_i = \frac{E_i \alpha_i}{\rho_i C_i} T_{0i}$ and $\lambda_i = \frac{\kappa_i}{\rho_i C_i}$.

Boundary conditions should be added at the outer boundary (i.e. for $y = y_1$ and $y = y_{N+1}$) and at each interface ($y = y_{i+1}$ with $i = 1,\ldots, N-1$). In this work we assume adiabatic boundary conditions at $y = y_1$ and $y = y_{N+1}$ while at the interfaces a linear combination of the temperature and of its normal derivative is prescribed together with the continuity of the heat flux:

$$
\begin{aligned}
&\frac{\partial T_1}{\partial y}=0 \quad \text{at } y=y_1\\
&-\kappa_i\frac{\partial T_i}{\partial y}=\varphi_{i+1}(T_i-T_{i+1}) \quad \text{and} \quad \kappa_i\frac{\partial T_i}{\partial y}=\kappa_{i+1}\frac{\partial T_{i+1}}{\partial y} \quad \text{at } y=y_{1+1} \qquad i=1,\dots N-1\\
&\frac{\partial T_N}{\partial y}=0 \quad \text{at } y=y_N
\end{aligned} \tag{8}
$$

The parameter φ_i characterizes the thermal behavior of the interface. For $\varphi_i \to \infty$ the case of thermally perfect interface is obtained, while $\varphi_i = 0$ corresponds to an adiabatic interface.

2.2 *Thermoelastic quality factor for three-layer symmetric resonators*

As shown by Zener [2] the thermoelastic quality factor can be computed as the ratio between the elastic deformation energy and the dissipated energy during harmonic vibrations. To this purpose the above formulated coupled thermoelastic problem should be solved for the case of harmonic vibrations of the form:

$$
\begin{aligned}
v(x,t) &= V(x)e^{i\omega t}\\
T(y,t) &= \mathcal{T}(y)e^{i\omega t}
\end{aligned} \tag{9}
$$

A particular configuration of a symmetric three-layer beam (Figure 2) will be considered, in view of its relevance in real MEMS resonators.

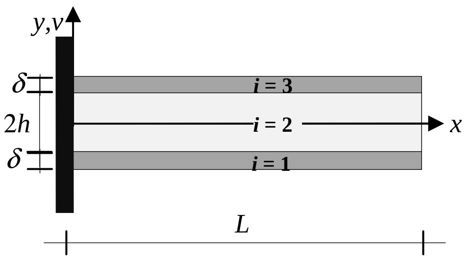

Figure 2: Schematic representation of a three-layer beam.

Taking into account the symmetry, only the part with $y > 0$ can be considered. Using (9), the heat conduction problem (7)-(8) specializes to

$$
\begin{aligned}
&i\omega\mathcal{T}_2 = i\omega\beta_2\frac{d^2V}{dx^2}y+\lambda_2\frac{\partial^2\mathcal{T}_2}{\partial y^2} \qquad 0<y<h\\
&i\omega\mathcal{T}_3 = i\omega\beta_3\frac{d^2V}{dx^2}y+\lambda_3\frac{\partial^2\mathcal{T}_3}{\partial y^2} \qquad h<y<h+\delta\\
&\text{b. c.}: \begin{cases}\mathcal{T}_2=0 \quad \text{at } y=0\\ -\kappa_2\dfrac{\partial\mathcal{T}_2}{\partial y}=\varphi(\mathcal{T}_2-\mathcal{T}_3) \quad \text{and} \quad \kappa_2\dfrac{\partial\mathcal{T}_2}{\partial y}=\kappa_3\dfrac{\partial\mathcal{T}_3}{\partial y} \quad \text{at } y=h\\ \dfrac{\partial\mathcal{T}_2}{\partial y}=0 \quad \text{at } y=h+\delta\end{cases}
\end{aligned} \tag{10}
$$

The solution in terms of temperature is sought in the form of series of eigenfunctions [9]:

$$\mathcal{T}_i = \sum_{n=1}^{\infty} G_n \psi_{in} = \sum_{n=1}^{\infty} G_n \left[A_{in} \sin\frac{\zeta_n y}{\sqrt{\lambda_i}} + B_{in} \cos\frac{\zeta_n y}{\sqrt{\lambda_i}} \right] \tag{11}$$

By introducing Eq. (11) into the boundary conditions (10), one obtains the following homogeneous linear system for the unknowns A_{in}, B_{in}:

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 \\ -H\zeta_n \cos\gamma\zeta_n - \sin\gamma\zeta_n & H\zeta_n \sin\gamma\zeta_n - \cos\gamma\zeta_n & \sin\frac{h}{h+\delta}\eta\zeta_n & \cos\frac{h}{h+\delta}\eta\zeta_n \\ K\cos\gamma\zeta_n & -K\sin\gamma\zeta_n & -\cos\frac{h}{h+\delta}\eta\zeta_n & \sin\frac{h}{h+\delta}\eta\zeta_n \\ 0 & 0 & \cos\eta\zeta_n & \sin\eta\zeta_n \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} A_{2n} \\ B_{2n} \\ A_{3n} \\ B_{3n} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

The following parameters have been introduced:

$$H = \frac{\kappa_2}{\varphi\sqrt{\lambda_2}};\ K = \frac{\kappa_2\sqrt{\lambda_3}}{\kappa_3\sqrt{\lambda_2}};\ \gamma = \frac{h}{2\sqrt{\lambda_2}};\ \eta = \frac{h+\delta}{2\sqrt{\lambda_3}} \tag{13}$$

The eigenvalues ζ_n can be found by imposing that det($\mathbf{C}$) = 0; consequently, a possible solution of the linear system can be found by imposing that $B_{2n} = 1$. The field equations (10) become:

$$\begin{aligned} i\omega\sum_{n=1}^{\infty} G_n \psi_{2n} &= i\omega\beta_2 \frac{d^2V}{dx^2} y + \lambda_2 \sum_{n=1}^{\infty} G_n \frac{\partial^2 \psi_{2n}}{\partial y^2} \qquad 0 < y < h \\ i\omega\sum_{n=1}^{\infty} G_n \psi_{3n} &= i\omega\beta_3 \frac{d^2V}{dx^2} y + \lambda_3 \sum_{n=1}^{\infty} G_n \frac{\partial^2 \psi_{3n}}{\partial y^2} \qquad h < y < h+\delta \end{aligned} \tag{14}$$

The following simple operations should now be performed: multiplication of the equations times $\kappa_i \psi_{ir}/\lambda_i$; integration of each equation over the layer thickness; addition of the l.h.s. and r.h.s. of all equations. Account taken of the eigenfunction properties [7]:

$$\sum_{i=1}^{N} \frac{\kappa_i}{\lambda_i} \int_{y_i}^{y_{i+1}} \psi_{in}\psi_{ir}\, dy = \begin{cases} 0 \text{ if } n \neq r \\ N_n \text{ if } n = r \end{cases} \qquad \frac{\partial^2 \psi_{in}}{\partial y^2} = -\frac{\zeta_n^2}{\lambda_i}\psi_{in} \tag{15}$$

one obtains the following set of decoupled equations, which easily yield the values G_n:

$$i\omega N_n G_n = i\omega\Gamma_n \frac{d^2V}{dx^2} - \zeta_n^2 N_n G_n \qquad \Gamma_n = \frac{\kappa_2\beta_2}{\lambda_2}\int_0^h \psi_{2n}\, y\, dy + \frac{\kappa_3\beta_3}{\lambda_3}\int_h^{h+\delta} \psi_{3n}\, y\, dy \tag{16}$$

The introduction of Eqs. (9) and (11) into the dynamic equilibrium equation (6), account taken of the values G_n obtained via Eq. (16), yields the following fourth order differential equation:

$$-V\omega^2 A+i\left[\sum_{n=1}^{\infty}\frac{\omega\zeta_n^2}{\omega^2+\zeta_n^4}\frac{\Gamma_n^*\Gamma_n}{N_n}\right]\frac{d^4V}{dx^4}+\left[I+\sum_{n=1}^{\infty}\frac{\omega\zeta_n^2}{\omega^2+\zeta_n^4}\frac{\Gamma_n^*\Gamma_n}{N_n}\right]\frac{d^4V}{dx^4}=0 \tag{17}$$

In the above equation, due to thermal coupling, the second dissipative term arises. The following parameters have been introduced for the sake of clarity

$$A=2[\rho_2 h+\rho_3\delta];\quad I=2\left[E_2\int_0^h y^2dy+E_3\int_h^{h+\delta}y^2dy\right];\quad \Gamma_n^*=2\left[\frac{\kappa_2\beta_2}{T_{02}\lambda_2}\int_0^h\psi_{2n}ydy+\frac{\kappa_3\beta_3}{T_{03}\lambda_3}\int_h^{h+\delta}\psi_{3n}ydy\right] \tag{18}$$

From Zener's definition [2], the quality factor is computed as follows:

$$Q=\frac{I+\sum_{n=1}^{\infty}\frac{\omega\zeta_n^2}{\omega^2+\zeta_n^4}\frac{\Gamma_n^*\Gamma_n}{N_n}}{\sum_{n=1}^{\infty}\frac{\omega\zeta_n^2}{\omega^2+\zeta_n^4}\frac{\Gamma_n^*\Gamma_n}{N_n}} \tag{19}$$

It is worth mentioning that the interface dissipation φ influences, through the parameter H in Eq. (12), the eigenvalues ζ_n, the eigenvector components and, consequently, the values N_n, Γ_n, Γ^*_n. If one sets $H = 0$ (i.e. if a thermally perfect interface is considered), the analytical results obtained in [6] and [9] are recovered by an alternative formulation.

3 RESULTS AND DISCUSSION

This Section summarizes the results of some of the performed analyses, in order to assess the effect of interface dissipation on micro-resonators. In all the cases, silicon cantilever are considered with different coating materials. It is important to remind the physical and mechanical properties of the different materials (Table 1); special attention should be paid to the quantity Ψ_0, which represents the maximum achievable thermo-elastic damping for homogeneous resonators. The maximum dissipation (and, as a consequence, the minimum quality factor Q_0) is achieved for beams whose resonance frequency equals the relaxation frequency:

$$f_0=\frac{\pi(\kappa/\rho C)}{2h_{tot}^2} \tag{20}$$

	E GPa	ρ kg/m^3	C J/(kg · K)	k W/(m · K)	α K^{-1}	T_0 K	Q_0	Ψ_0
Si	160	2330	690	150	2.6E-6	300	9860	6.37E-4
Cu	120	8900	430	400	2.0E-5	300	530	1.19E-2
SiC	400	3200	940	70	3.0E-6	300	5560	1.13E-3
SiO_2	70	2150	740	1.3	5.0E-7	300	60610	1.04E-5

Table 1: Physical and mechanical properties of the materials adopted in the examples

3.1 *Laminated Cu-Si-Cu resonators*

The first examples are referred to three-layer beams with silicon core and copper skins. The thickness of the Si layer is kept constant and equal to 2μm; the volume fraction of copper, with respect to the overall thickness, is $V_f = 0.1$, which means that the Cu layers are 0.11μm thick. By considering Table 1, it is possible to conclude that copper is by far more dissipative than silicon. Figure 3 shows the preliminary results for thermally perfect interface. As expected, the graph (which are in agreement with the ones reported in [6]) shows that the laminated resonators are more dissipative than bare silicon beams. The pairwise correspondent symbols refer to beams of different length and show a slight reduction of natural frequencies for the layered resonators.

Figure 4 shows the effect of interface dissipation. The most intriguing result is represented by the appearance of a peak of damping for a particular value of φ. For $\varphi \to \infty$ the solution for perfect interface is recovered; the case $\varphi \to 0$ refers to adiabatic interface, which correspond to independent thermal vibration of the layers and to lower dissipation. The interaction of the two thermal modes yields the dissipation peak, whose value seems to be roughly independent of the beam length.

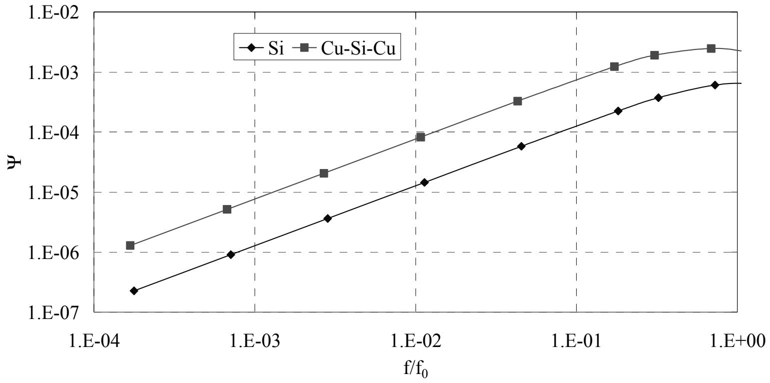

Figure 3: Thermoelastic damping for Cu-Si-Cu resonators with thermally perfect interface ($V_f = 0.1$) compared to bare Si resonators. Thickness of the Si layer is $2h$ = 2μm. f_0 = 37MHz is referred to bare Si beams. Beams of various length, from 10μm to 640μm, correspond to symbols.

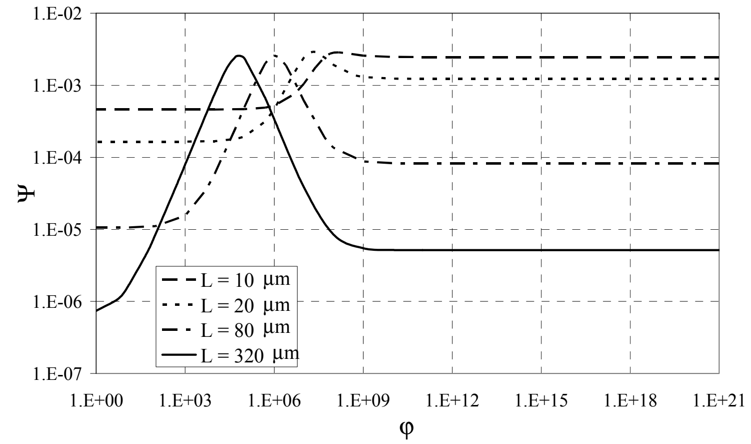

Figure 4: Thermoelastic damping vs. interface dissipation parameter in Cu-Si-Cu beams ($V_f = 0.1$).

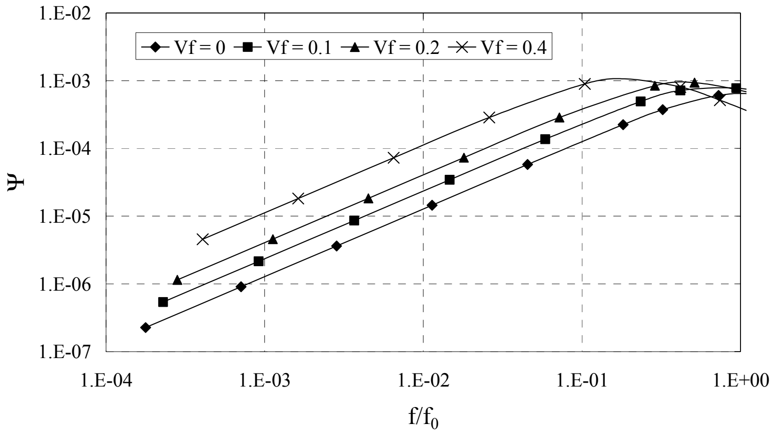

Figure 5: Thermoelastic damping for SiC-Si-SiC resonators with thermally perfect interface and various volume fractions V_f. Thickness of the Si layer is $2h$ = 2μm. f_0= 37MHz is referred to bare Si beams. Beams of various length, from 10μm to 640μm, correspond to symbols on the curves.

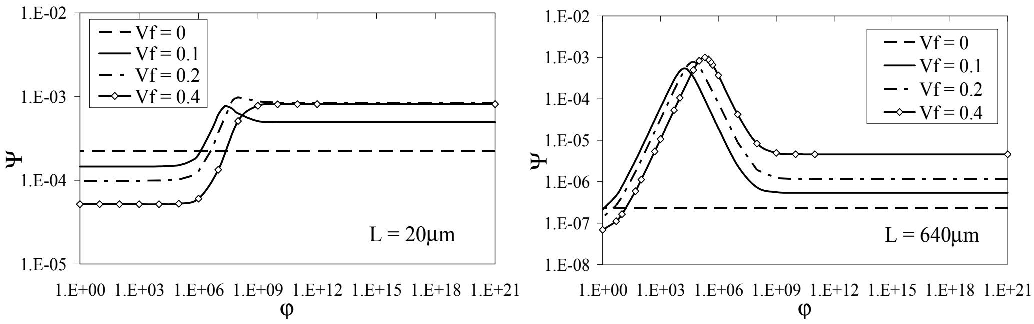

Figure 6: Thermoelastic damping vs. interface dissipation parameter for SiC-Si-Sic resonators (left hand side L = 20μm, right hand side L = 640μm). Thickness of the Si layer is $2h$ = 2μm.

3.2 *Laminated SiC-Si-SiC resonators*

The case of silicon beams with silicon carbide coatings is now considered. The Si core is 2μm thick. The deposition of SiC layers entails a strong increase of resonance frequency (as shown by the symbols in Figure 5, referred to thermally perfect interface). Even for such resonators, the material in the skins is endowed with higher intrinsic damping: consequently, one would expect that the higher the volume fraction, the higher the dissipation. This is true only in the low-frequency region, where the damping for V_f = 0.4 is increased by a factor 20 with respect to bare Si; conversely, for high frequencies, a reduction of Ψ is observed, as shown also in [6].

The results for dissipative interface are reported in Figure 6. The graph on the left is referred to high-frequency resonators (f = 6.69MHz for bare Si, f/f_0 = 0.182): a non-monotonic trend for dissipation is confirmed. Moreover, the dissipation peak seems to disappear in case of high volume fractions. A totally different picture is sketched on the right part, which refers to resonators in the tens-of-kHz range (f = 26kHz for bare Si, f/f_0 = 7.10E-4). The dissipation peak is evident for any volume fraction, with increase of 3-4 orders of magnitude. It is important to notice that the maximum dissipation is quite similar for the various thicknesses of SiC layers. This confirms, qualitatively, the experimental results obtained by Sandberg et al. [8], who evidenced that the deposition of a thin layer yields a significant increase of dissipation; further growth of the coating thickness leads only to a small variation of damping.

3.3 *Oxidized resonators.*

An important problem is represented by “nominally” homogeneous Si beams, which actually are covered by a very thin layer of oxide (SiO_2). For perfect interface, given the intrinsic dissipation of SiO_2, the oxidized resonators should be less dissipative than pure silicon. Figures 7 and 8 show what happens for dissipative interface. For high-frequency beams, the dissipation peak is low; moreover, the increase of oxide thickness corresponds to a decrease of damping. When examining low-frequency resonators, one observes that the presence of thermal jump at the interface gives rise, even for very thin oxide layer, to a significant increase of damping. In the latter case, thicker oxide layers produce a steady increase of dissipation. Finally, as shown in Figure 8, the dissipation peak, that is almost absent for short beams, reaches a constant value for longer beams. This result, summarized in Figure 9, is of special importance if one considers the experimental measurements for ultra-thin resonators, reported e.g. in [1]. In that paper, a constant dissipation threshold, significantly higher than Zener’s prediction, is observed.

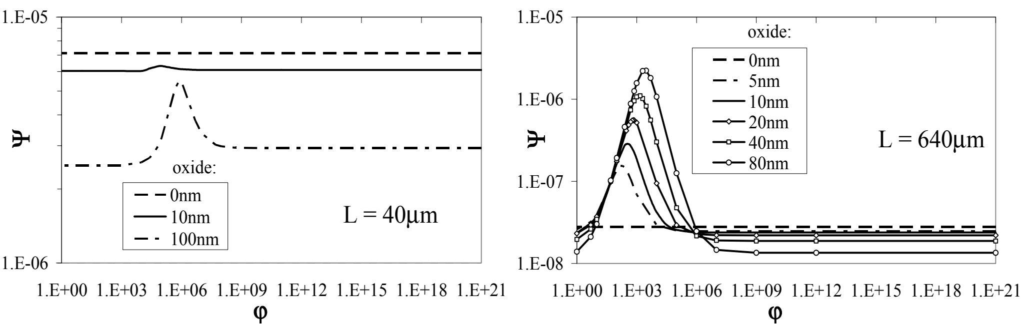

Figure 7: Thermoelastic damping vs. interface dissipation parameter for oxidized resonators (left hand side L = 40µm, right end side L = 640µm). Thickness of the beams is $2h$ = 1µm..

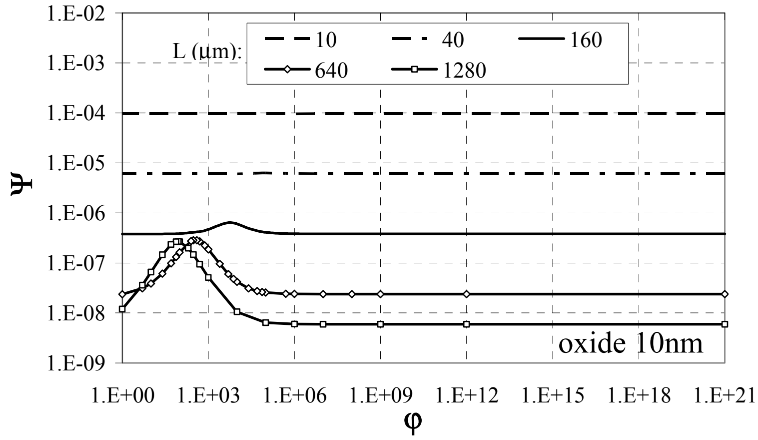

Figure 8: Thermoelastic damping vs. interface dissipation parameter for oxidized resonators of various length. Oxide layer is 10nm thick. Thickness of the beams is $2h$ = 1µm..

4 CONCLUSIONS

The problem of thermoelastic damping for layered resonators has been considered, taking into account the presence of dissipative interfaces between the layers. The analytical treatment of the problem has furnished a simple procedure for the evaluation of quality factor Q, for the special case of three-layer beams. Extension to different cases is straightforward and will be considered in a future paper. From the proposed examples, it has been highlighted the effect of interface dissipation, which could explain the experimental results for coated cantilevers and oxidized ultra-thin resonators. The encouraging results will spur further research on these points.

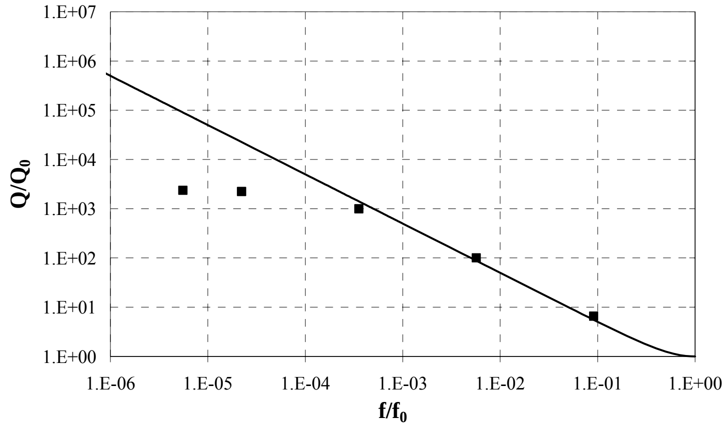

Figure 9: Quality factor of oxidized Si resonators of various length, with dissipative interface at dissipation peak (squares), compared to Zener's solution (solid line). Oxide layer is 10nm thick. Thickness of the beams is $2h$ = 1μm. f_0 and Q_0 are referred to non-oxidized Si beams.

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