Finite Element Modeling of the Thermoelastic Damping in Micro-Electromechanical Systems*

S. Lepage†, J.C. Golinval

University of Liege, Vibrations and Identification of Structures,
Chemin des Chevreuils, 1, B52, B-4000 Liege, Belgium

Abstract

In the design of micro-electromechanical systems, which require a high quality factor, the dissipation mechanisms such as the thermoelastic damping have to be considered. In order to assess the thermoelastic influence on the behavior of vibrating structures, analytical models may be used for simple configurations under very restrictive assumptions. In order to study more complex structures, the finite element method may be used. Two simple cases for which analytical models exist are investigated in this paper. An oscillating clamped-clamped beam and a vibrating bar are modelled using thermoelastic finite elements. The analytical and finite element analyses show that the thermoelastic coupling implies a natural frequency shift, an amplitude attenuation, a difference of phase between the thermal and mechanical degrees of freedom and influences the quality factor of the resonating system.

Keywords:
Finite elements, thermoelastic coupling, thermoelastic damping, micro-structures.

1 Introduction

In order to design resonant micro-systems with high quality factors, dissipation mechanisms have to be minimized. Air damping, anchor damping, electronics damping and thermoelastic damping have been identified as important loss mechanisms in micro-resonators [1]. However, few predictive damping modeling techniques exist. This may be explained by the wide variety of damping sources. Sorting out the various mechanisms is not straightforward. External sources of damping, such as dissipation at interfaces or induced by the surrounding environment, are difficult to model. However, these external sources of dissipation can be avoided or at least decreased by modifying the system. For example, air damping can be eliminated by packaging the mechanism under vacuum. Thermoelastic damping, which may be classified as an internal source of dissipation, may be predicted analytically [2-4]. However, the models found in the literature are based on very restrictive assumptions and can only be used for simple configurations. In order to investigate structures of more complex geometry, a numerical approach is required. The first part of this paper presents the analytical models. Then, the finite element formulation for thermoelastic problems is exposed. Finally, the developed F.E. formulation is validated on two simple examples, for which analytical solutions are available. The first example considers the axial vibrations of a bar, while the second one studies the vibrations of a beam in flexion.

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†Corresponding author. E-mail: SLepage@ulg.ac.be.

2 Analytical models

Physically, thermoelastic damping represents the loss in energy from an entropy rise caused by the coupling between heat transfer and strain rate. Indeed, in isotropic solids with a positive thermal expansion coefficient, an increase of temperature creates a dilation and inversely, a decrease of temperature produces a compression. Similarly, a dilation lowers the temperature and a compression raises the temperature. Therefore, when a thermoelastic solid is set in motion, it is taken out of equilibrium, having an excess of kinetic and potential energy. The coupling between the strain and the temperature fields induces an energy dissipation mechanism which causes the system to return to its static equilibrium. The relaxation of the thermoelastic solid is achieved through the irreversible flow of heat driven by local temperature gradients that are generated by the strain field. This dissipation effect is not always measurable. When the vibration frequency is much lower than the relaxation rate, the solid is always in thermal equilibrium and the vibrations are isothermal. On the other hand, when the vibration frequency is much higher than the relaxation rate, the system has no time to relax and the vibrations are adiabatic. Hence, it is only when the vibration frequency is of the order of the relaxation rate that the energy loss becomes appreciable.

2.1 Zener's standard model

Zener [4] has developped expressions to approximate the thermoelastic damping. His theory is based on an extension of Hooke's law involving stress σ, strain ε as well as their first time derivatives $\dot{\sigma}$ and $\dot{\varepsilon}$ [4]:

$$\sigma + \tau_\varepsilon \dot{\sigma} = E_R(\varepsilon + \tau_\sigma \dot{\varepsilon}) \tag{2.1}$$

This model is called the "Standard Anelastic Solid" model. The three parameters τ_ε, τ_σ and E_R have the following physical interpretation:

- τ_ε is the relaxation time at which the stress relaxes exponentially when the strain is kept constant.
- τ_σ is the relaxation time at which the strain relaxes exponentially when the stress is kept constant.
- E_R is the elastic modulus after all relaxations occurred.

The unrelaxed value of the elastic modulus E_U can be defined using the three previous parameters:

$$E_U = E_R \frac{\tau_\sigma}{\tau_\varepsilon} \tag{2.2}$$

In order to analyze the vibration characteristics of the solid, the stress and the strain are considered to vary harmonically at the natural pulsation ω_n. The dissipation in the solid can be measured by Q^{-1}, the inverse of the quality factor of the resonating beam, which is defined as the fraction of energy lost per cycle:

$$Q^{-1} = \Delta_E \frac{\omega_n \tau}{1 + (\omega_n \tau)^2} \tag{2.3}$$

where $\tau = \sqrt{\tau_\sigma \tau_\varepsilon}$ is the effective relaxation time and $\Delta_E = \sqrt{\frac{\tau_\sigma}{\tau_\varepsilon}} - \sqrt{\frac{\tau_\varepsilon}{\tau_\sigma}} = \frac{E_U - E_R}{\sqrt{E_R E_U}}$ is the relaxation strength.

Thus, the dissipation exhibits a Lorentzian behavior as a function of $\omega_n \tau$ with a maximum value of $\Delta_E/2$ when $\omega_n \tau = 1$. This agrees with the previous qualitative explanation. When the frequency is small compared to the relaxation rate, $\omega_n \tau << 1$ and the thermoelastic dissipation is negligible as the oscillations are isothermal. On the other hand, when the frequency is large compared to the relaxation rate, $\omega_n \tau >> 1$ and the oscillations are adiabatic. Therefore, it is only when the frequency is of the order of the relaxation rate, i.e. $\omega_n \tau \approx 1$, that the thermoelastic dissipation takes importance.

For a beam in flexion, assuming that the relaxation occurs only through the first transverse conduction mode and that the thermoelastic natural frequency ω_n can be approximated by the isothermal frequency $\omega_{o,n}$, the inverse of the quality factor for a thermoelastic flexural beam resonator can be expressed as follows

$$Q^{-1} = \frac{E\alpha^2 T_o}{C_v} \frac{2\zeta^2/\pi^2}{1 + (2\zeta^2/\pi^2)^2} \tag{2.4}$$

where E is the Young modulus, α is the heat expansion coefficient, C_v is the heat capacity at constant volume, T_o is the reference temperature and ζ is a dimensionless parameter which depends on the thermal diffusivity $\chi = \kappa/C_v$ where κ is the thermal conductivity, the beam thickness b and the isothermal frequency $\omega_{o,n}$: $\zeta = b\sqrt{\frac{\omega_{o,n}}{2\chi}}$.

The quality factor of a bar in axial vibrations has the same expression as equation (2.4) if it is assumed that the relaxation occurs only through the first longitudinal thermal mode and that the thermoelastic frequency can be approximated by its isothermal value. However, for a bar in axial vibrations, b is replaced by l, which is the bar length.

According to equation (2.4), the influence of the thermoelastic coupling on the quality factor is maximum when $2\zeta^2/\pi^2 = 1$. Hence, the importance of the thermoelastic effects depends on the material thermal and mechanical properties as well as on the dimensions of the structure. It can be shown that for a clamped-clamped beam in silicon, the thermoelastic damping is maximum when the beam thickness and length satisfy the equation: $b^3/l^2 = 1.8\ 10^{-8}$ m. When $b^3/l^2 >> 1.8\ 10^{-8}$ m, the beam is in adiabatic regime and inversely, when $b^3/l^2 << 1.8\ 10^{-8}$ m, the beam is in isothermal regime. On the other hand, for a bar in silicon fixed at its center and free at its ends, the thermoelastic effects are maximum when its length is $3.4\ 10^{-8}$ m. In practice, bars are usually largely longer than $3.4\ 10^{-8}$ m so that they are in adiabatic regime.

2.2 Solutions of the thermoelastic equations for harmonic vibrations

The effects of the thermoelastic coupling do not only affect the quality factor but also influence the resonance frequency. Although the change in the resonance frequency induced by the thermoelastic coupling can be neglected in most cases, it has to be taken into account in the design of frequency-agile applications, e.g. micro-resonators. Zener's theory [3], exposed previously, does not allow to estimate the frequency shift induced by thermoelastic effects. The resolution of the equations of linear thermoelasticity allows to assess the expression of the complex thermoelastic pulsation ω_n. The real part $\Re(\omega_n)$ gives the new resonant pulsation of the beam in the presence of thermoelastic coupling. The frequency shift can be calculated by $(\Re(\omega_n) - \omega_{o,n})/\omega_{o,n}$. The imaginary part $\Im(\omega_n)$ induces an amplitude attenuation of the vibration, which is quantified by $\Im(\omega_n)/\omega_{o,n}$.

Assuming that there is no longitudinal thermal relaxation, Lifshitz and Roukes [2] obtained an expression for the complex thermoelastic pulsation for the flexion of a rectangular beam:

$$\Re(\omega_n) = \omega_{o,n}\left[1 + \frac{\Delta_E}{2}\left(1 - \frac{6}{\zeta^3}\frac{\sinh\zeta - \sin\zeta}{\cosh\zeta + \cos\zeta}\right)\right] \tag{2.5}$$

$$\Im(\omega_n) = \omega_{o,n}\frac{\Delta_E}{2}\left(\frac{6}{\zeta^3}\frac{\sinh\zeta + \sin\zeta}{\cosh\zeta + \cos\zeta} - \frac{6}{\zeta^2}\right) \tag{2.6}$$

Similarly, the complex pulsation of an axially vibrating bar can be assessed from the linear thermoelastic equations. Assuming that the mechanical and thermal modes are not modified due to the thermoelastic coupling, the thermoelastic pulsation of a bar fixed at its center and free at both ends satisfies the following equation:

$$-\frac{\rho}{E}\left(\frac{l}{\pi}\right)^2 i\omega_n^3 - \frac{\rho}{E}\left(\frac{l}{\pi}\right)^4 \frac{\kappa}{C_v}\omega_n^2 + \left(1 + \frac{T_o\alpha^2 E}{C_v}\right) i\omega_n + \frac{\kappa}{C_v}\left(\frac{l}{\pi}\right)^2 = 0 \tag{2.7}$$

It should be noted that the thermal mode used considers that the temperature is fixed at both ends, which is in agreement with the mechanical boundary conditions.

The quality factor can be expressed in terms of the imaginary and real parts of the frequency. The inverse of the quality factor, which is the fraction of energy lost per radian, is given by

$$\begin{aligned} Q^{-1} &= \frac{2\left|\Im(\omega_n)\right|}{\sqrt{\Re^2(\omega_n) + \Im^2(\omega_n)}} && (2.8)\\ &\approx 2\left|\frac{\Im(\omega_n)}{\Re(\omega_n)}\right| && (2.9)\end{aligned}$$

as the imaginary part of the resonant pulsation can be considered to be small compared to the real part.

3 Finite Element Formulation

The analytical models are based on very restrictive assumptions and can only be used for simple configurations such as a beam in flexion or a bar in extension. In order to investigate structures of more complex geometry, a numerical approach is required. The finite element method is a powerful technique, which provides solutions to many complex problems and is widely used in engineering design.

The thermoelastic finite element formulation can be derived from Hamilton's variational principle in which both mechanical and thermal degrees of freedom are considered simultaneously. The displacement field $\mathbf{u}$ and the temperature increment θ are related to the corresponding node values $\mathbf{u_u}$ and $\mathbf{u}_\theta$ by the mean of shape function matrices $\mathbf{N_u}$ and $\mathbf{N}_\theta$

$$\begin{aligned} \mathbf{u} &= \mathbf{N_u}\mathbf{u_u} && (3.10)\\ \theta &= \mathbf{N}_\theta\mathbf{u}_\theta && (3.11)\end{aligned}$$

Therefore, the strain field $\boldsymbol{\varepsilon}$ and the thermal field $\mathbf{e}$ are related to the vectors of degrees of freedom through the shape function derivative matrices $\mathbf{B_u}$ and $\mathbf{B}_\theta$

$$\begin{aligned} \boldsymbol{\varepsilon} &= \mathcal{D}\mathbf{N_u}\mathbf{u_u} = \mathbf{B_u}\mathbf{u_u} && (3.12)\\ \mathbf{e} &= -\nabla\mathbf{N}_\theta\mathbf{u}_\theta = \mathbf{B}_\theta\mathbf{u}_\theta && (3.13)\end{aligned}$$

where ∇ is the gradient operator and $\mathcal{D}$ is the derivation operator defined so that $\varepsilon = \mathcal{D}\mathbf{u}$ according to the displacement compatibility equation. Hence, the dynamic equilibrium equation governing the thermoelastic problem is:

$$\begin{pmatrix} \mathbf{M_{uu}} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \ddot{\mathbf{u}}_{\mathbf{u}} \\ \ddot{\mathbf{u}}_{\theta} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \mathbf{C}_{\theta\mathbf{u}} & \mathbf{C}_{\theta\theta} \end{pmatrix}\begin{pmatrix} \dot{\mathbf{u}}_{\mathbf{u}} \\ \dot{\mathbf{u}}_{\theta} \end{pmatrix} + \\ + \begin{pmatrix} \mathbf{K_{uu}} & \mathbf{K}_{\mathbf{u}\theta} \\ 0 & \mathbf{K}_{\theta\theta} \end{pmatrix}\begin{pmatrix} \mathbf{u}_{\mathbf{u}} \\ \mathbf{u}_{\theta} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{\mathbf{u}} \\ \mathbf{F}_{\theta} \end{pmatrix} \tag{3.14}$$

where $\mathbf{M_{uu}}$ is the mass matrix, $\mathbf{C}_{\theta\mathbf{u}}$ is the damping matrix due to the thermo-mechanical coupling effect and $\mathbf{C}_{\theta\theta}$ is the damping matrix due to the thermal field. The matrix $\mathbf{K}_{\mathbf{u}\theta}$ is the stiffness matrix due to the thermo-mechanical coupling. Matrices $\mathbf{K_{uu}}$ and $\mathbf{K}_{\theta\theta}$ are the stiffness matrices due to mechanical and thermal fields, respectively. Vectors $\mathbf{F_u}$ and $\mathbf{F}_\theta$ are the force vectors due to mechanical and thermal fields, respectively.

As explained in section 2, the thermoelastic coupling modifies the quality factor of the response, induces both damping and resonance frequency shift. Equation (3.14) takes the general form

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{C}\dot{\mathbf{q}} + \mathbf{K}\mathbf{q} = 0 \tag{3.15}$$

where $\mathbf{C}$ and $\mathbf{K}$ are non-symmetric matrices. This problem may be transformed into a linear problem of twice the size through a linearization procedure. Partitioning the eigenvectors into thermal and mechanical degrees of freedom and substituting the time derivative of the thermal degrees of freedom by their values, the eigenvalue problem to solve may be rewritten in the form

$$\begin{pmatrix} -\mathbf{K}_{uu} & -\mathbf{K}_{u\theta} & 0 \\ 0 & -\mathbf{K}_{\theta\theta} & 0 \\ 0 & 0 & \mathbf{M}_{uu} \end{pmatrix}\begin{pmatrix} \mathbf{x}_u \\ \mathbf{x}_\theta \\ \dot{\mathbf{x}}_u \end{pmatrix} = \lambda \begin{pmatrix} 0 & 0 & \mathbf{M}_{uu} \\ \mathbf{C}_{\theta u} & \mathbf{C}_{\theta\theta} & 0 \\ \mathbf{M}_{uu} & 0 & 0 \end{pmatrix}\begin{pmatrix} \mathbf{x}_u \\ \mathbf{x}_\theta \\ \dot{\mathbf{x}}_u \end{pmatrix} \tag{3.16}$$

If the number of mechanical and thermal degrees of freedom is denoted n_u and n_θ, respectively, the eigenvalue problem (3.16) has $2n_u$ conjugate complex eigenvalues and n_θ real eigenvalues. The $2n_u$ eigenvalues correspond to the mechanical eigenfrequencies and the n_θ ones to the thermal eigenfrequencies.

Based on the thermoelastic finite element formulation, bar and beam elements have been developed. The degrees of freedom of the bar element correspond to the temperature increment and to the axial displacement at the end nodes. The beam elements are based on the Euler-Bernoulli assumption and have two thermal and two mechanical degrees of freedom per node. The thermal degrees of freedom correspond to the temperature increment and the transverse thermal gradient at the neutral axis of the beam. These elements assume that the transverse temperature distribution is a cubic function of the thickness and that the upper and lower surfaces are thermally insulated. Both bar and beam elements use linear shape functions for the longitudinal variation of both the displacement and the temperature.

4 Applications

The finite element formulation developed in this work has been validated on two simple examples, for which analytical solutions are available. The first example considers the axial vibrations of a bar, which is fixed at its center and free at its ends; moreover, the temperature at its ends is fixed to the ambient temperature. The second example consists in a vibrating clamped-clamped beam in which the transverse thermoelastic relaxation is studied. The thermal boundary conditions impose a fixed temperature at the ends of the neutral fibre of the beam. Moreover, the upper and lower surfaces are considered to be thermally insulated as assumed in the thermoelastic beam finite element formulation. The material considered is silicon, as it is largely used in micro-technology. Its thermal and mechanical properties are: $E = 1.65810^{11}\ N/m^2$, $\nu = 0.2$, $\rho = 2300\ kg/m^3$, $c_v = 711\ J/kgK$, $\alpha = 2.510^{-6}\ K^{-1}$ and $\kappa = 170\ Wm^{-1}K^{-1}$.

4.1 Axial vibration of a bar

As discussed in section 2, thermoelastic damping is maximum when the length of the bar is equal to 3.4 10^{-8}m. In practice, this dimension is too small. This is the reason why thermoelastic effects are studied here for bars whose length varies from 0.5 μm to 1000 μm.

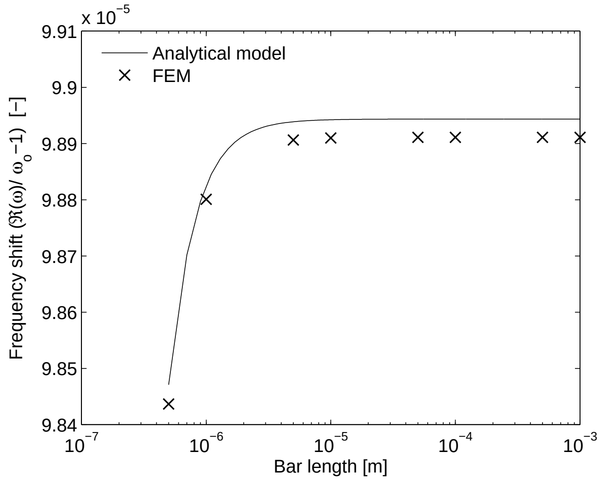

Figure 4.1: Variation of the frequency shift versus the bar length.

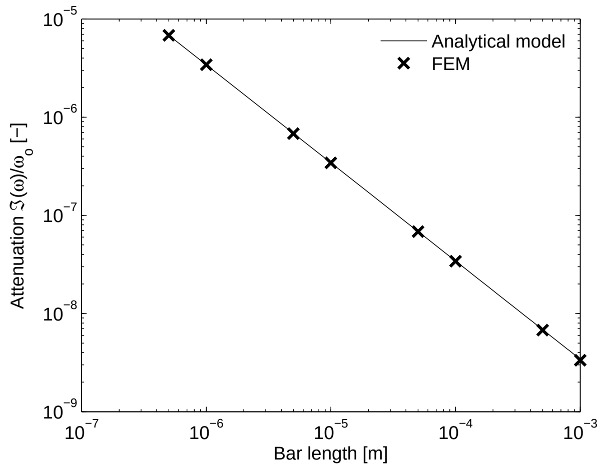

Figure 4.2: Variation of the amplitude attenuation versus the bar length.

Figures 4.1 and 4.2 represent the variation of the frequency shift and the amplitude attenuation versus the bar length. When the length is larger than 5 μm, the frequency shift remains constant and the bar can be considered to be in adiabatic regime. Moreover, for large bar lengths, the amplitude attenuation is less than 10^{-7}, which is negligible in most applications. Figure 4.3 shows the variation of the quality factor for different bar lengths. It is observed that the thermoelastic quality factor varies linearly with the bar length. All these results show that the analytical models and the finite element simulations are in good agreement.

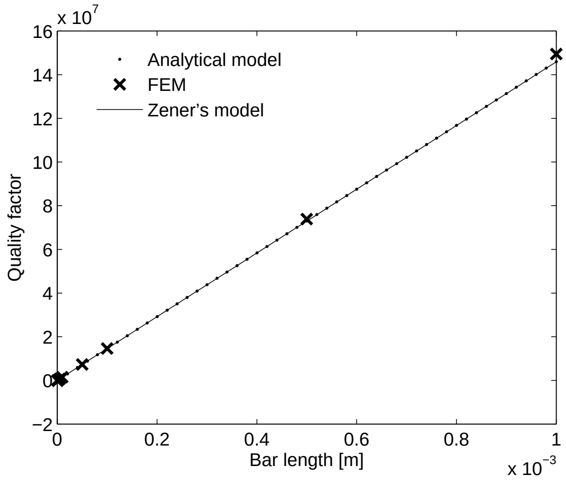

Figure 4.3: Variation of the inverse of the quality factor of the axial vibration of a beam.

4.2 Bending of a clamped-clamped beam

As stated by the analytical models, the thermoelastic effects on the behavior of an oscillating beam depend on the aspect ratio of the beam. Indeed, the thermoelastic effects are maximum when $h^3/l^2 = 1.8\ 10^{-8}$m. In this example, they are investigated for a beam of 90 μm length and for different beam thicknesses. According to the analytical model, for a beam length of 90 μm, the thickness for which the thermoelastic damping is maximum is 5.3 μm. Therefore, the beam thickness is varied from 3 μm to 9 μm, while the beam width is fixed to 4.5 μm.

Figure 4.4 represents the variation of the frequency shift and the amplitude attenuation. It is observed that the frequency shift increases with the thickness of the beam. For small beam thicknesses, the frequency shift is nought, i.e. the beam behavior is isothermal. When the beam thickness becomes large enough, the slope decreases so that the frequency shift tends to reach an upper limit of 7.5 10^{-5}, which is the frequency shift between the adiabatic and isothermal values. The amplitude attenuation presents a maximum value of 4 10^{-5} for a beam thickness of 5.3 μm, i.e. the beam thickness for which the thermoelastic effects are maximum according to the analytical models. Figure 4.5 shows the variation of the inverse of the quality factor $Q^{-1} = \left|2\frac{\Im(\omega_n)}{\Re(\omega_n)}\right|$ with the thickness of the beam. The inverse of the quality factor reaches a maximum of 7.9 10^{-5} for a beam thickness of 5.3 μm as predicted by the analytical model.

Thermoelasticity introduces complex eigenfrequencies and complex eigenmodes. Thermal and mechanical degrees of freedom are found to be out of phase. It means that the maximum of the temperature increment does not occur when the deformation is maximum. This is due to the relaxation which occurs through heat conduction. The difference of phase between the thermal and mechanical degrees of freedom depends on the magnitude of the thermoelastic effects as shown in figure 4.6.

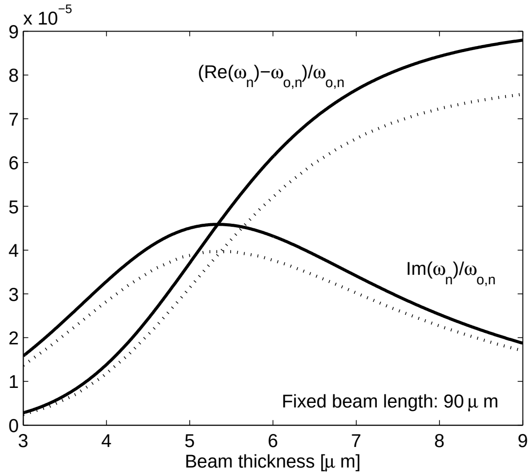

Figure 4.4: Variation of the frequency shift and attenuation with the thickness (FEM: dotted line, Analytical model: solid line).

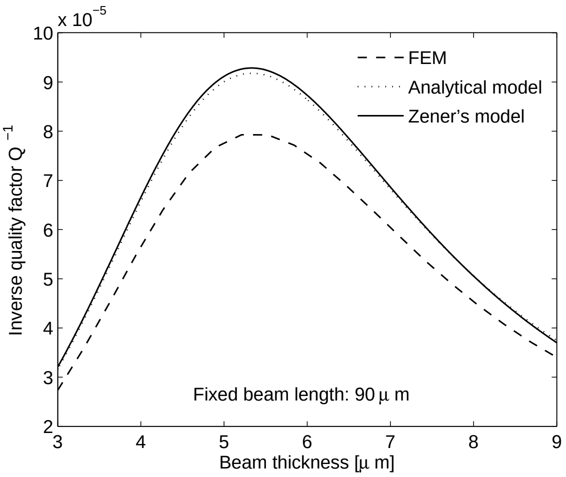

Figure 4.5: Variation of the inverse of the quality factor.

The analytical and finite element models gives similar results even if the finite element results are smaller than the analytical ones. However, the beam thickness for which the thermoelastic effects are maximum is the same in both approaches. The difference between the analytical and finite element results can be explained by the different inherent assumptions on which they are based. Indeed, the finite element model assumes that the tranverse temperature variation is a cubic function while in the analytical formulation, the thermal modes are trigonometric functions when they are not influenced by thermoelastic coupling. Another difference lies in the fact that the analytical models neglect the longitudinal thermal relaxation. However, this assumption is not too restrictive as the longitudinal thermoelastic effects are negligible for a length of 90 μm.

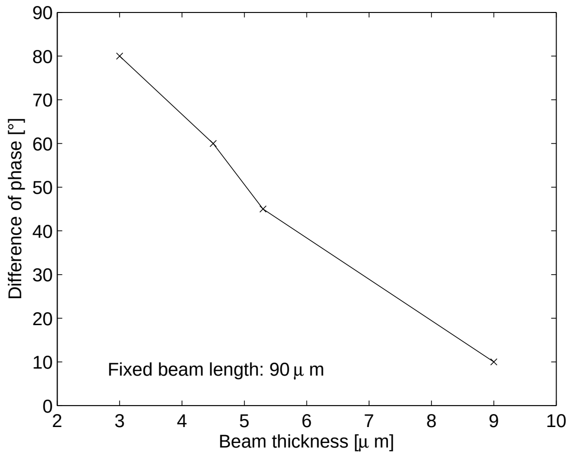

Figure 4.6: Variation of the difference of phase between the thermal and mechanical degrees of freedom.

5 Conclusion

In order to assess the thermoelastic influence on the behavior of micro-structures, thermoelastic finite element simulations were carried out on two simple cases for which analytical results are available. The analytical and finite element models give similar results. They show that thermoelastic coupling implies a shift in the natural frequency, an amplitude attenuation and modifies the quality factor of the resonant device. Moreover, the finite element analysis allows to quantify the difference of phase between the thermal and mechanical degrees of freedom. It is also shown that the importance of the thermoelastic effect depends on the dimensions of the micro-structure (e.g. length of the bar).

The development of thermoelastic finite elements will allow to consider the study of complex structures in the future and to quantify the influence of parameters such as the thermal boundary conditions on the quality factor of micro-resonators.

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