

## Multimode thermoelastic dissipation

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In this paper, we investigate thermoelastic dissipation (TED) in systems whose thermal response is characterized by multiple time constants. Zener [Phys. Rev. **52**, 230 (1937)] analyzed TED in a cantilever with the assumption that heat transfer is one dimensional. He showed that a single thermal mode was dominant and arrived at a formula for quantifying the quality factor of a resonating cantilever. In this paper, we present a formulation of thermoelastic damping based on entropy generation that accounts for heat transfer in three dimensions and still enables analytical closed form solutions for energy loss estimation in a variety of resonating structures. We apply this solution technique for estimation of quality factor in bulk mode, torsional, and flexural resonators. We show that the thermoelastic damping limited quality factor in bulk mode resonators with resonator frequency much larger than the eigenfrequencies of the dominant thermal modes is inversely proportional to the frequency of the resonator unlike in flexural mode resonators where the quality factor is directly proportional to the resonant frequency. Purely torsional resonators are not limited by TED as the deformation is isochoric. We show that it is possible to express the quality factor obtained by full three-dimensional analyses as a weighted sum of Zener formula based modal quality factors. We analytically estimate the quality factor of a cantilever and a fixed-fixed beam and corroborate it with data to show that the assumption of a single dominant thermal mode, which is valid in one-dimensional analysis, is violated. The analytical formulation described in this paper permits estimation of energy lost due to heat transfer in orthogonal directions. It is found that the entropy generated due to heat transfer along the beam becomes significant in beams with aspect ratio (length/width) below 20. © 2009 American Institute of Physics. [DOI: 10.1063/1.3072682]

### I. INTRODUCTION

Understanding energy loss mechanisms is critical for the design of mechanical dynamical systems. A microresonator is an example of a microelectromechanical system (MEMS) whose performance is governed by energy dissipation. Air damping, clamping losses, and thermoelastic dissipation (TED) are some of the energy loss mechanisms that prevail in microresonators. Air damping involves transfer of energy from the vibrating structure to air molecules. Clamping loss refers to the irretrievable energy transmitted to the supporting structure of the vibrating structure. TED refers to the energy lost due to relaxation of temperature distribution resulting from applied strain field. Zener<sup>1</sup> studied and modeled TED in cantilevers in 1937. In recent years, TED has been revisited primarily because its effects are encountered in MEMS devices,<sup>2–19</sup> and there is much interest in improving the computational approaches for resonator design, in particular, the impact of TED.

In the original paper by Zener,<sup>1</sup> the phenomenon of TED was analyzed for a one-dimensional case, specifically in a cantilever beam. Zener calculated the temperature field developed in the cantilever due to the periodic strain field by expanding the solution in terms of thermal modes, eigenfunctions of Helmholtz equation for a one-dimensional system. Using the temperature field, he calculated the bending

moment caused by the temperature gradient in the cantilever. Relaxation of the thermal gradient due to heat transfer results in a bending moment component that is 90° out of phase to work done on the cantilever. By determining this contribution, he calculated the energy lost in the system. The four primary assumptions in the derivation of the final result were as follows. (1) The quality factor of the resonating device is very high thereby precluding effects on resonant frequency due to quality factor. (2) The mechanical and thermal equations are weakly coupled, whereby the temperature field generated by the strain does not significantly affect the dynamic behavior of the mechanical system because the temperature rise is very small. (3) The first mode contributes significantly more than other modes to the energy loss. (4) The heat transfer occurs only across one dimension. Zener arrived at a formula involving sum of Lorentzians each of which captured the contribution of several thermal modes. He showed that the contribution of the first thermal mode was much larger than the rest of the modes thereby coming to a formula involving a single Lorentzian

$$Q^{-1} = \underbrace{\frac{\alpha^2 E T_{\text{reservoir}}}{c_v}}_{\text{material term}} \underbrace{\frac{\omega \tau_{\text{th}}}{1 + (\omega \tau_{\text{th}})^2}}_{\text{frequency term}}, \quad (1)$$

where  $Q$  is the quality factor of the resonant cantilever beam,  $E$  is Young's modulus of the material,  $\alpha$  is the thermal coefficient of expansion,  $c_v$  is the heat capacity per unit volume,

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$T_{\text{reservoir}}$  is the temperature of the thermal reservoir connected to the beam,  $\omega$  is the frequency of vibration of the beam,  $\tau_{\text{th}}$  is the diffusion time,  $w$  is the width of the beam, and  $k$  is the thermal conductivity of the material. In this paper, we will refer to this formula as the Zener formula.

The simplicity of this formula lies in the separation of a material property dependent term and the thermal time constant dependent term embodied in the Lorentzian. Owing to this simplicity, efforts have been made to describe energy loss in complex structures with multiple thermal time constants, such as slots in beam structures<sup>7</sup> and polycrystalline silicon,<sup>13</sup> by adding inverse quality factors by using an amended Zener formula. A more sophisticated version of Zener's formula for TED estimation was derived by Lifshitz and Roukes<sup>17</sup> which took into account the fact that the resonant frequency of the structure has a slight dependence on quality factor. Analytical solution for estimation of TED in laminated structures has also been investigated.<sup>20</sup> This analytical solution was obtained following similar analysis as Zener, retaining the assumption that the heat transfer in the structure is one dimensional. De and Aluru<sup>8</sup> investigated the effect of nonlinearity introduced by electrostatic actuation on thermoelastic damping. Other flexural beamlike geometries such as a ring resonator vibrating in a wine glass mode have also been investigated.<sup>5</sup>

It was recently recognized that a fully coupled solution

can be obtained using currently available computational resources.<sup>21</sup> This solution technique forgoes both the assumptions made by Zener and deals with a general case. However, by retaining only the first assumption made by Zener in his analysis, a semianalytical solution that offers insight into the physics to a greater extent can be derived for three-dimensional cases. In this paper, we describe an entropy generation based formulation. An entropy generation based formulation has been discussed by Bishop and Kinra<sup>20</sup> in the context of laminated structures and applied to beam structures. However, these formulations lead to a complex final solution form and are not amenable for analytical estimation of quality factor in a generic resonator. The solution technique presented in this paper will be illustrated through application of the analytical solution technique to quality factor estimation in bulk mode resonators, torsional resonators, and flexural resonators. We will also investigate the correctness of the assumptions of heat transfer along one dimension, presence of a single dominant thermal mode, and suitability of amending Zener's formula for complex geometries.

## II. THEORY

### A. Definitions

Quality factor is a measure of energy loss in a resonator. Formally, it is defined as

$$Q = 2\pi \frac{\text{maximum energy stored during a period of oscillation}}{\text{energy lost during a period of oscillation}}. \quad (2)$$

For heat conduction, entropy generation per unit volume, a strictly positive quantity, is given by<sup>22</sup>

$$\dot{S}_{\text{generation}} = k \frac{\nabla T \cdot \nabla T}{T^2}, \quad (3)$$

where  $\dot{S}_{\text{generation}}$  is the rate of entropy generation and  $T$  is the temperature of the unit volume. Energy loss can be thermodynamically quantified using lost work. By Gouy–Stodola theorem,<sup>22</sup> the rate of lost work per unit volume is related to entropy generation and the temperature of the thermal reservoir connected to the resonator system as given by

$$\dot{W}_{\text{lost}} = T_{\text{reservoir}} \dot{S}_{\text{generation}} = T_{\text{reservoir}} k \frac{\nabla T \cdot \nabla T}{T^2}, \quad (4)$$

where  $\dot{W}_{\text{lost}}$  is the lost work. Zener also derived an entropy based expression for the rate of lost energy per unit volume<sup>23</sup> as given by

$$\dot{Q}_{\text{lost}} = T_{\text{reservoir}} \frac{k \nabla^2 T}{T}, \quad (5)$$

where  $\dot{Q}_{\text{lost}}$  is the rate of heat loss. It can be shown that Eqs. (4) and (5) are equivalent when integrated over the entire volume by invoking first Green's identity.

In the discussion that follows, we will calculate the energy lost in system by calculating the spatial overlap between the mechanical modes and thermal modes. The eigensolutions of the vibration equations will be referred to as mechanical modes. The eigenvalue corresponding to a mechanical mode is a measure of frequency of vibration. Figure 1(a) shows the boundary conditions of a simple beam and Figs. 1(b) and 1(c) show the first and third mechanical modes of this structure. In solving homogeneous heat equation with time invariant physical properties given by

$$k \nabla^2 T = c_v \frac{\partial T}{\partial t} \quad (6)$$

using separation of variables, one encounters the Helmholtz equation (7).

$$k \nabla^2 v_i(x, y, z) + \lambda_i c_v v_i(x, y, z) = 0,$$

$$\int_V v_i(x, y, z) d\Omega = V, \quad (7)$$

where  $v_i$  is the eigensolution and  $\lambda_i$  is the eigenvalue. We will refer to these normalized eigensolutions ( $v_i$ ) of Eq. (7) as thermal modes. It is convenient to use thermal modes as basis functions to expand solutions of general heat equation

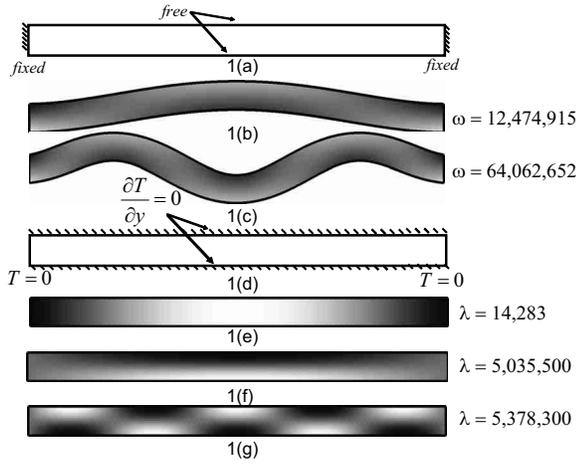


FIG. 1. Thermal modes and mechanical modes. (a) Structural boundary conditions of a fixed-fixed beam. [(b) and (c)] First and third mechanical vibration modes along with the mode frequencies of a fixed-fixed beam of dimensions  $12 \times 200 \mu\text{m}^2$ . The dark regions correspond to large volumetric changes. (d) Thermal boundary conditions of a fixed-fixed beam. [(e)–(g)] Thermal modes of a fixed-fixed beam. The dark shaded regions correspond to temperatures higher than the reservoir temperature and the bright regions correspond to temperatures lower than the reservoir temperature.

because the eigenfrequency corresponding to each thermal mode represents the decay time constant of each mode. Figure 1(d) shows the boundary conditions of a simple beam structure which has a constant temperature at two of its ends and is insulated at the other two and Figs. 1(e)–1(g) show three representative thermal modes of this structure.

## B. Thermoelastic dissipation equations: Formulation and solution methods

Before formulating the TED equations, it is instructive to delve into the cause of temperature change induced by an applied strain. Zener<sup>1</sup> derived an expression for the change in temperature due to strain using Maxwell identities of thermodynamics. Here, we present an alternate approach based on entropy to find the change in the temperature of a body due to change in its volume. This approach relates fundamental phonon physics to the macroscopically calculated heat source term, thus revealing that the energy loss in materials is governed by their overall Grüneisen parameter.

Consider a simple body that is adiabatically sealed at its surface. When a reversible force is applied, work is performed on the body. By first law of thermodynamics, the internal energy of the body increases. However, a tensile force causes a temperature decrease while a compressive force causes a temperature increase in the body. To explain this, one has to resort to the second law of thermodynamics. When the volume of a solid is increased the entropy of the body tends to increase. However, since the applied force was reversibly applied and the body is adiabatically sealed, this process is isentropic. In order to compensate the increase in the entropy due to volume increase, the temperature of the body reduces. Thus, tensile strain results in temperature reduction in the body. Likewise, compressive strain tends to reduce the entropy of the body which gets compensated by an increase in temperature. This fact, derived in Appendix A, is expressed mathematically as

$$\left(\frac{\partial T}{\partial V}\right)_s = -\frac{T}{V}\gamma, \quad (8)$$

where the left hand side term represents the change in temperature due to change in volume at constant entropy and  $\gamma$  is overall Grüneisen's parameter.<sup>24</sup> Furthermore, overall Grüneisen's parameter<sup>15</sup> is related to the thermal coefficient of expansion ( $\alpha$ ), bulk modulus ( $B$ ), and heat capacity at constant volume ( $c_v$ ) as given by

$$\alpha = \frac{\gamma c_v}{3B}. \quad (9)$$

It is shown in Appendix A that the effect of applied strain manifests as a heat source term in the heat equation

$$c_v \frac{\partial T}{\partial t} = k \nabla^2 T - \underbrace{3\alpha BT \left[ \frac{\partial}{\partial t} \left( \frac{\delta V}{V} \right) \right]}_{\text{heat source}}. \quad (10)$$

Here,  $[\partial/\partial t(\delta V/V)]$  is the rate change in volumetric change at each point in the solid. If the change in temperature is not significant compared to the temperature of the heat reservoir connected to the resonating structure, the heat source term is independent of the change in temperature to the first order. Then, a linear transformation  $T = T_{\text{reservoir}} + \theta$  yields

$$c_v \frac{\partial \theta}{\partial t} = k \nabla^2 \theta - 3\alpha B T_{\text{reservoir}} \left[ \frac{\partial}{\partial t} \left( \frac{\delta V}{V} \right) \right]. \quad (11)$$

In the following discussion, we will investigate multi-mode TED wherein several thermal modes contribute significantly to entropy production. This analysis approach, while retaining the complexity induced by three-dimensional nature of the problem, allows for a simple semianalytical solution. We find that the quality factor can be expressed as a weighted sum of Lorentzians corresponding to each thermal mode and that the weights depend on the spatial overlap of the mechanical and thermal modes.

To solve Eq. (11), we first need to solve for the displacement solution of the vibration equations. The general time harmonic steady periodic solution of vibration equations has the form given by

$$\left(\frac{\delta V}{V}\right) = \varepsilon_V(x, y, z) \sin(\omega t), \quad (12)$$

where  $\varepsilon_V(x, y, z)$  is the spatial function describing the amplitude of volumetric change in the solid. Using Eq. (12), the heat source term in Eq. (11) can be expressed as a product of a spatial term and a time harmonic term.

$$q = \underbrace{-3\alpha B T_{\text{reservoir}} \omega \varepsilon_V(x, y, z)}_{\text{spatial component: } q(x, y, z)} \times \underbrace{\cos(\omega t)}_{\text{temporal component}}. \quad (13)$$

In order to solve Eq. (11), it is convenient to project the spatial component of the heat source term ( $q(x, y, z)$ ) on the thermal modes ( $v_i$ ) of the system as

$$\begin{aligned}
 q(x, y, z) &= \sum 3\alpha BT_{\text{reservoir}} \omega a_i v_i(x, y, z) \\
 &= \sum 3\alpha BT_{\text{reservoir}} \omega \underbrace{\left( \frac{1}{3\alpha BT_{\text{reservoir}} \omega} \frac{\int_V q(x, y, z) v_i(x, y, z) d\Omega}{\int_V v_i^2(x, y, z) d\Omega} \right)}_{a_i} v_i(x, y, z)
 \end{aligned} \tag{14}$$

The magnitude of the overlap integrals  $a_i$  depends on the overlap of spatial distribution of strain and the corresponding thermal mode. If the displacement is normalized such that

$$\int_V \left( \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z} \right)^2 d\Omega = V, \tag{15}$$

then the overlap integrals ( $a_i$ ) in Eq. (14) satisfy the property

$$\sum_i a_i^2 = 1. \tag{16}$$

Let the temperature change  $\theta$  be expressed as a sum of products of time dependent coefficients  $g_i$  and thermal modes  $v_i(x, y, z)$ ,

$$\theta = \sum g_i(t) v_i(x, y, z). \tag{17}$$

Upon substituting Eqs. (17) and (6) into Eq. (11) and noting that the thermal modes are orthogonal to each other, a set of ordinary differential equations is obtained.

$$\dot{g}_i + \lambda_i g_i = 3\alpha BT_{\text{reservoir}} \frac{a_i}{c_v} \omega \cos(\omega t). \tag{18}$$

The steady periodic solution of Eq. (18) takes the form

$$g_i(t) = -3\alpha BT_{\text{reservoir}} \frac{a_i}{c_v} \frac{\omega}{\sqrt{\lambda_i^2 + \omega^2}} \sin \left[ \omega t + \tan^{-1} \left( \frac{\lambda_i}{\omega} \right) \right]. \tag{19}$$

Substituting Eqs. (19) and (17) into Eq. (3), one obtains an expression for entropy generation per unit time per unit volume.

$$\begin{aligned}
 \dot{S}_{\text{generation}} &= \frac{k}{T_{\text{reservoir}}} \sum_j \sum_i g_i(t) g_j(t) \left( \frac{\partial v_i}{\partial x} \frac{\partial v_j}{\partial x} + \frac{\partial v_i}{\partial y} \frac{\partial v_j}{\partial y} \right. \\
 &\quad \left. + \frac{\partial v_i}{\partial z} \frac{\partial v_j}{\partial z} \right).
 \end{aligned} \tag{20}$$

An initial look at Eq. (20) suggests that the expression for entropy generated will involve coupled terms between various thermal modes. However, at this point we invoke the fact that the thermal modes are orthogonal to each other and so are their spatial gradients. Thus, upon integration of Eq. (20) over one period of vibration and spatial domain of the vibrating structure, one obtains a simple expression for entropy generation.

$$(S_{\text{generation}})_{\text{tot}} = \sum_i \underbrace{\frac{9\pi\alpha^2 B^2}{c_v}}_{\text{material term}} \underbrace{a_i^2}_{\text{spatial overlap}} \underbrace{\frac{\omega\lambda_i}{\omega^2 + \lambda_i^2}}_{\text{mechanical frequency term}}. \tag{21}$$

Here, we invoked the fact that when the boundary conditions are homogeneous, gradients of eigenfunctions are orthogonal to each other. Upon substituting Eq. (21) into Eq. (3), we find the lost work ( $W_{\text{lost}}$ ).

$$\begin{aligned}
 W_{\text{lost}} &= T_{\text{reservoir}} \sum_i \frac{9\pi\alpha^2 B^2}{c_v} a_i^2 \frac{\omega\lambda_i}{\omega^2 + \lambda_i^2} \\
 &= 9\pi \frac{B^2}{E} \sum_i a_i^2 \frac{\alpha^2 E T_{\text{reservoir}}}{c_v} \frac{\omega\lambda_i}{\omega^2 + \lambda_i^2}.
 \end{aligned} \tag{22}$$

Thus, quality factor for a multimode system is arrived at by substituting Eq. (22) into Eq. (1),

$$\begin{aligned}
 Q^{-1} &= \frac{1}{2\pi} \frac{W_{\text{lost}}}{W_{\text{stored}}} \\
 &= \frac{9}{2} \frac{B^2}{E W_{\text{stored}}} \sum_i a_i^2 \underbrace{\left( \frac{\alpha^2 E T_{\text{reservoir}}}{c_v} \frac{\omega\lambda_i}{\omega^2 + \lambda_i^2} \right)}_{\text{Zener's formula based modal quality factor}} \\
 &= \frac{9}{2} \frac{B^2}{E W_{\text{stored}}} \sum_i a_i^2 Q_i^{-1},
 \end{aligned} \tag{23}$$

where  $W_{\text{stored}}$  is the total energy stored in the resonator and  $Q_i$  is a Zener formula based modal quality factor. The energy stored in a resonator made of linear elastic material is given by

$$\begin{aligned}
 W_{\text{stored}} &= \phi E, \\
 \phi &= \frac{(1-\nu)}{2(1-2\nu)(1+\nu)} \int_V \left\{ \left[ \left( \frac{\partial u_1}{\partial x} \right)^2 + \left( \frac{\partial u_2}{\partial y} \right)^2 + \left( \frac{\partial u_3}{\partial z} \right)^2 \right] \right. \\
 &\quad \left. + \frac{2\nu}{1-\nu} \left( \frac{\partial u_1}{\partial x} \frac{\partial u_2}{\partial y} + \frac{\partial u_2}{\partial y} \frac{\partial u_3}{\partial z} + \frac{\partial u_3}{\partial z} \frac{\partial u_1}{\partial x} \right) \right\} dV.
 \end{aligned} \tag{24}$$

Here  $\phi$  is the proportionality constant that relates the energy stored in a resonator and the elastic modulus. The value of this constant needs to be determined given the displacement solution of the vibration equations and the constraint equa-

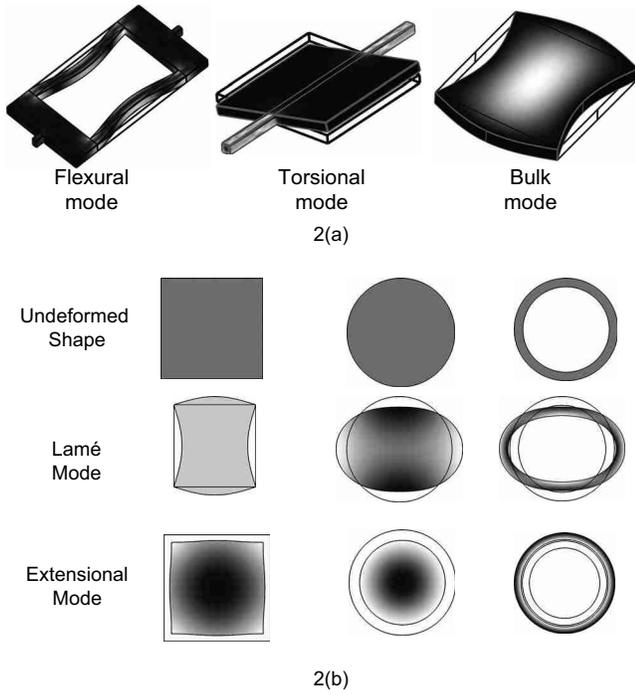


FIG. 2. (a) Three types of mechanical resonators: flexural mode, torsional mode, and bulk mode. (b) Bulk mode resonators with different geometries and mode of operation.

tion (15). Substituting Eq. (24) into Eq. (23) and relating bulk modulus with Young's modulus, we find a simple expression for quality factor in terms of modal Zener quality factors and weighting coefficients  $b_i$ ,

$$Q^{-1} = \sum_i b_i Q_i^{-1},$$

$$b_i = \frac{1}{2} \frac{1}{\phi(1-2\nu)^2} a_i^2. \quad (25)$$

Thus the overall quality factor limited by TED can be seen to be expressed as a weighted sum of modal Zener quality factors. In Sec. III, we employ this entropy based formulation to obtain analytical expressions for energy loss in three types of mechanical resonators, viz., flexural resonators, bulk mode resonators, and torsional resonators. The result in Eq. (25) emphasizes the need for appropriate estimation of the weighting factor and is surprisingly simple considering that it is valid for an arbitrary three-dimensional geometry. In Sec. III, we obtain analytical solutions for quality factor of various mode shapes and geometries of resonators.

### III. ANALYTICAL ESTIMATION OF QUALITY FACTOR

The commonly employed resonator designs can be broadly classified as per their mode of operation, namely, flexural, torsional, and bulk mode devices [Fig. 2(a)]. In the flexural devices, the principal stress is approximately aligned with the normal stress along the structure and is orthogonal to the linear displacement of the flexure. Flexural vibration modes can be viewed as transverse standing waves. The dominant stress in torsional resonators is shear stress and the displacement is rotational while bulk mode devices are char-

acterized by normal stresses that are aligned parallel to the displacement of the structure and are representative of longitudinal transverse waves. An exception to this common aspect of bulk mode structures is the Lamé mode wherein the displacement at the center of the edges is orthogonal to the dominant normal stress. Figure 2(b) shows the commonly used bulk mode device design shapes such as square plate, circular disk, and ring that may be operated in extensional (contour) and Lamé modes.

#### A. Bulk mode resonators

We first estimate the energy loss due to TED in bulk mode resonators. The bulk mode resonator shapes are typically characterized by a single dimension. For instance, a square resonator is characterized by the length of the edge, a disk and a ring by their radii, and a beam by its length. The natural frequency and thermal modes of these resonators depend on the material properties and the characteristic length of the resonator. The natural frequency of bulk mode resonators typically takes the form

$$\omega = c_\omega \frac{1}{L} \sqrt{\frac{E}{\rho}}, \quad (26)$$

where  $E$  is the elastic modulus,  $\rho$  is the density of the structure,  $L$  is a characteristic length scale of the bulk mode resonator, and  $c_\omega$  is a constant of proportionality. The thermal mode frequencies of the bulk mode resonators take the form

$$\lambda_i = c_\lambda \frac{k_{\text{thermal}}}{c_v} \frac{1}{L^2}, \quad (27)$$

where  $c_\lambda$  is a constant of proportionality. In the case of bulk mode resonators, the thermal mode frequencies are typically much smaller than the resonant frequency of the device; i.e.,  $\lambda_i/\omega \ll 1$ . Thus, Eq. (23) takes the form

$$Q^{-1} \approx \frac{9}{2} \pi T_{\text{reservoir}} \frac{\alpha^2 B^2}{c_v} \sum_i a_i^2 \frac{\lambda_i}{\omega}. \quad (28)$$

Substituting Eqs. (26) and (27) into Eq. (28), we obtain after appropriate mathematical manipulation of resulting expression an expression for  $Q_{\text{TED,bulk}}$  in terms of its mechanical resonant frequency.

$$Q_{\text{TED,bulk}} = \frac{1}{\psi} \frac{c_v^2}{\alpha^2 \rho k_{\text{thermal}} T_{\text{reservoir}} \omega}. \quad (29)$$

This expression, though quite general, does depend on the specific design of the bulk mode structure through the constant  $\psi$ . In Secs. III A 1–III A 3 we obtain an analytical expression for the constant  $\psi$  for the cases of a square resonator in extensional mode and Lamé mode, a ring resonator in first and second extensional modes, and a disk resonator in extensional mode. We finally discuss the thermoelastic damping limited quality factor of one of the commonly employed bulk mode structures, an extensional mode of a beam fixed at one end, and show that the frequency dependence is different from other bulk modes for this vibration mode.

### 1. Square resonator: Extensional and Lamé modes

We next consider a square resonator of side  $L$  which has been attached only at one end by a flimsy spring that allows the resonator to move freely in extensional mode and Lamé mode. For the extensional mode of the square resonator, we approximate the displacement solution as<sup>25</sup>

$$U = w_0 \sin \pi \xi,$$

$$V = w_0 \sin \pi \eta, \quad (30)$$

where  $\xi = x/L$  and  $\eta = y/L$  are dimensional coordinates that vary from  $-1/2$  to  $+1/2$ . The resonant frequency of the extensional mode as estimated by Rayleigh's energy method is given by

$$\omega = \frac{1}{L} \sqrt{\frac{(1-\nu)(\pi^2 + 8\nu)E}{(1+\nu)(1-2\nu)\rho}}. \quad (31)$$

The change in volume can then be estimated to be

$$\varepsilon_V(\xi, \eta) = w_0 \pi (\cos \pi \xi + \cos \pi \eta). \quad (32)$$

The edges of the square are insulated and thus, the thermal modes of this structure are

$$\nu(m, n) = 2 \sin \pi \xi (2m + 1) \sin \pi \eta (2n + 1),$$

$$\lambda(m, n) = \frac{k}{c_v} \pi^2 \left[ \left( \frac{2m + 1}{L} \right)^2 + \left( \frac{2n + 1}{w} \right)^2 \right]. \quad (33)$$

It can be shown that the thermal modes in Eq. (33) are orthogonal to the expression in Eq. (32). Thus, to the first order, TED in square extensional resonators is negligible. It should be noted, however, that the solution for the displacement assumed in Eq. (30) is approximate. Analysis of extensional mode of a square resonator using a finite element method based technique followed by the application of the entropic method outlined in Sec. II allows estimation of the constant  $\psi$ . However, the dependence on Poisson's ratio is not preserved in the numerical estimation. For silicon with Poisson's ratio of 0.22, the constant  $\psi$  is

$$\psi_{\text{extensional mode square}} = 6.33. \quad (34)$$

Next we consider the Lamé mode of the square resonator. The displacement solution of the Lamé mode can be approximated by<sup>26</sup>

$$u = \cos \pi \xi \sin \pi \xi \eta,$$

$$v = -\sin \pi \xi \cos \pi \eta. \quad (35)$$

where  $\xi = x/L$  and  $\eta = y/L$  are dimensional coordinates that vary from 0 to 1.

It can be shown that the volumetric change in this mode is uniformly zero,

$$\varepsilon_V(\xi, \eta) = 0. \quad (36)$$

Thus, the Lamé mode of a square resonator is uniformly isochoric. Using Eq. (13), we can see that there is no heat

generation at any point of the resonator. Thus, TED is negligible in the Lamé mode of the square resonator and the constant  $\psi$  is zero for this mode,

$$\psi_{\text{Lamé mode square}} = 0. \quad (37)$$

### 2. Ring resonator: Extensional mode

We now consider a ring resonator whose inner radius is  $R_1$  and outer radius is  $R_2$ . We further assume that the thickness of the ring is much smaller than the radius, i.e.,  $t = R_1 - R_2 \ll R_1$ . We consider the extensional mode of this resonator. The displacement solution is approximately given by

$$u_r = u_0,$$

$$u_\theta = 0, \quad (38)$$

where  $u_r$  is the displacement in the radial direction and  $u_\theta$  is the displacement in the tangential direction. The corresponding change in volume is

$$\varepsilon_V(r, \theta) = \frac{u_0}{r} (1 - \nu) \approx \frac{u_0}{\left( \frac{R_1 + R_2}{2} \right)} (1 - \nu). \quad (39)$$

With the assumption of a thin ring, the approximation in Eq. (39) is very accurate. The generation of heat in the structure in the extensional mode is uniform to the first order. Thus, the overlap of thermal modes with the spatial profile of the generated heat is minimal and the constant  $\psi$  in Eq. (29) is zero to the first order. Through numerical simulation, a value can be obtained for silicon (with  $\nu = 0.22$ ),

$$\psi_{\text{extensional mode ring}} = 6.33. \quad (40)$$

### 3. Disk resonator: Extensional and Lamé modes

Next we consider a disk resonator with radius  $R$  which vibrates in extensional mode in its plane. The displacement solution of this mode is given by

$$u_r = u_0 \sin \left( \frac{\pi}{2} \xi \right),$$

$$u_\theta = \frac{R}{1.4802} \left( \frac{1 - \nu}{1 - 2\nu} \right), \quad (41)$$

where  $\xi = r/R$  varies from 0 to 1. The frequency of vibration can be estimated using the Rayleigh energy method

$$\omega = \frac{1}{R} \sqrt{\frac{2.8464(1.191 + \nu)E}{(1 - \nu^2)\rho}}. \quad (42)$$

The change in volume in the disk in the extensional mode is

$$\varepsilon_V(\xi) = \frac{u_0}{R} \left[ \frac{\pi}{2} \cos\left(\frac{\pi}{2}\xi\right) + \frac{1}{\xi} \sin\left(\frac{\pi}{2}\xi\right) \right]. \quad (43)$$

The thermal modes of a disk are Bessel functions of first kind given by

$$v_i = \frac{\sqrt{2}}{J_2(z_{1i})} J_0(z_{1i}\xi),$$

$$\lambda_i = \frac{z_{1i}^2 k}{R^2 c_v}, \quad (44)$$

where  $J_i$  is the Bessel function of first kind of order  $i$  and  $z_{1i}$  are the zeros of  $J_1$ . In addition, there is another thermal mode whose eigenfrequency is zero and spatial distribution is constant,

$$v_0 = 1, \quad \lambda_0 = 0. \quad (45)$$

The overlap integrals cannot be found in a closed form manner and the numerically estimated values for first six thermal modes are as follows:

$$a_0 = 0.9554, \quad a_1 = 0.2833, \quad a_2 = 0.0717,$$

$$a_3 = 0.0330, \quad a_4 = 0.0190, \quad a_5 = 0.0123. \quad (46)$$

It is apparent that the large overlap with the constant thermal mode would minimize the energy loss as the constant thermal mode does not cause energy loss. The constant  $\psi$  can be estimated to be

$$\psi_{\text{extensional mode disk}} = 8.9087 \frac{(1 + \nu)^2}{(1.191 + \nu)^2}. \quad (47)$$

The energy loss in Lamé mode of the resonator can be estimated numerically and the value for the constant  $\psi$ ,

$$\psi_{\text{Lamé mode disk}} = 10.1. \quad (48)$$

#### 4. Fixed-free beam: Extensional mode

In all the cases of the bulk mode resonators considered in Secs. III A 1–III A 3, we found that the quality factor could be represented as per Eq. (29) with appropriately estimated constant  $\psi$ . We next consider the important case of an extensional mode vibration mode of a fixed-free beam and find that the quality factor needs to retain the sum of Lorentzians as given by Eq. (23).

Consider a beam of cross-section area  $A$  and length  $L$  fixed at one end and free at the other. The spatial distribution of the displacement and the resonant frequency of the  $r$ th extensional vibration mode of the resonator are given by

$$U = u_0 \sin(2r - 1) \frac{\pi}{2} \xi,$$

$$\omega = \left( \frac{2r - 1}{2} \right) \frac{\pi}{L} \sqrt{\frac{E}{\rho}}, \quad (49)$$

where  $U$  is the displacement of the beam and  $\xi = x/L$  is a dimensionless coordinate that varies from 0 to 1. Thus the gradient of displacement is given by

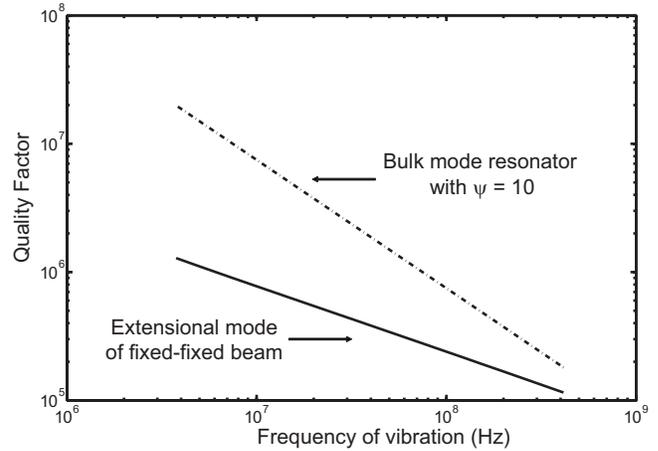


FIG. 3. Quality factor of a fixed-fixed beam vibrating in extensional mode and its comparison with a bulk mode resonator whose quality factor has a frequency dependence as given by Eq. (23) with  $\psi = 10$ . This value of  $\psi$  is close to that for most of the bulk mode resonant modes discussed in this paper.

$$\varepsilon_V(\xi) = u_0(2r - 1) \frac{\pi}{2L} \cos(2r - 1) \frac{\pi}{2} \xi. \quad (50)$$

Assuming that the beam vibrates in a vacuum environment, the beam has insulation along all the surfaces except at the base. If the beam is connected to a large temperature reservoir, the temperature of the beam at the base can be assumed to be constant. With these boundary conditions, the thermal modes of the beam can be obtained as

$$\nu(m) = \sqrt{2} \sin \pi \xi \left( \frac{2m - 1}{2} \right),$$

$$\lambda(m) = \frac{k}{c_v} \pi^2 \left( \frac{2m - 1}{2L} \right)^2, \quad (51)$$

where  $m$  takes on values from the set  $\{1, 2, 3, \dots\}$ . The overlap integrals  $a(r, m)$  can thus be obtained as

$$a(r, m) = (2r - 1) \frac{\pi}{2\sqrt{2}} \frac{(2r - 1)(-1)^r (-1)^m - (2m - 1)}{r^2 - r - m^2 + m}. \quad (52)$$

Unlike the other bulk modes, the summation term in Eq. (28) for the extensional mode of fixed-free beam does not converge. Thus, the quality factor for this case has to be determined by using the sum of Lorentzians

$$Q^{-1} \Big|_{\text{first extensional mode}} = \frac{(1 - 2\nu)(1 + \nu)}{(1 - \nu)(1 - 2\nu^2)} \frac{E\alpha^2 T_{\text{reservoir}}}{c_v}$$

$$\times \sum_m a(1, m) \frac{\lambda(m)/\omega}{1 + [\lambda(m)/\omega]^2}. \quad (53)$$

Figure 3 shows the frequency dependence of the quality factor of a fixed-free beam with variable length vibrating in the longitudinal extensional mode and compares the quality factor of a bulk mode structure whose quality factor is predicted by Eq. (23) with  $\psi=10$ .

## B. Torsional resonators

Pure torsion results in isochoric strain profile in structures. Thus, the heat generation due to the deformation is negligible in the resonator and hence, the energy loss due to TED is negligible.

## C. Flexural resonators

We consider two types of commonly encountered flexural resonators: fixed-free resonators and fixed-fixed resonators. For estimation of the quality factor using Eq. (23), it is sufficient to estimate the resonant frequency and the thermal mode frequencies ( $\lambda_i$ ) along with the corresponding overlap integrals ( $a_i$ ).

### 1. Fixed-free beam

Consider a cantilever beam of length  $L$  with a rectangular cross section ( $w \times t$ ) vibrating in a plane. Assuming that Euler–Bernoulli equations hold for the cantilever, the vibration mode of the beam<sup>27</sup> can be written as

$$u = u_0[\sin \beta \zeta - \sinh \beta \zeta - o(\cos \beta \zeta - \cosh \beta \zeta)],$$

where

$$a_i(m, n)_{\text{cantilever}} = 2(2.5429) \left( \frac{2(-1)^n}{\pi^2(2n+1)^2} \right) \left( \frac{\beta(-1)^{m+1} \cos(\beta) + o\beta(-1)^m \sin(\beta) + o\left(\frac{2m+1}{2}\right)\pi}{-\beta^2 + \left(\frac{2m+1}{2}\right)^2 \pi^2} \right. \\ \left. + \frac{\beta(-1)^{m+1} \cosh(\beta) + o\beta(-1)^m \sinh(\beta) + o\left(\frac{2m+1}{2}\right)\pi}{\beta^2 + \left(\frac{2m+1}{2}\right)^2 \pi^2} \right). \quad (57)$$

### 2. Fixed-fixed beam

Following similar method for a fixed-fixed beam, assuming that the displacement is given by

$$u = u_0[-\sin \beta \zeta + \sinh \beta \zeta - o(\cos \beta \zeta - \cosh \beta \zeta)],$$

where

$$o = \frac{\sin \beta + \sinh \beta}{\cos \beta + \cosh \beta}, \quad \beta = 1.875 \quad (\text{for first harmonic}), \\ \omega = \frac{\beta^2}{L^2} \sqrt{\frac{EI}{\rho A}}, \quad (54)$$

where  $u$  is the displacement of the cantilever,  $\zeta=x/L$  is a dimensionless coordinate that varies from 0 to 1,  $\beta$  is a constant associated with the mode of vibration, and  $\omega$  is the resonant frequency. Further assuming that the bending stress is the dominant stress and using the normalization condition for strain equation (15), the change in volume can be estimated to be

$$\nabla \cdot \vec{U} = 2.5429 \eta [-\sin \beta \zeta - \sinh \beta \zeta + o(\cos \beta \zeta + \cosh \beta \zeta)], \quad (55)$$

where  $\eta=y/w$  is a dimensional coordinate that varies from  $-1/2$  to  $+1/2$  and  $\nabla \cdot \vec{U}$  is the spatial distribution of change in volume of the resonator solid. The thermal boundary conditions for this cantilever are exactly similar to those of the beam discussed in Sec. III A 1.

$$\nu(m, n) = 2 \sin \pi \zeta \left( \frac{2m+1}{2} \right) \sin \pi \eta (2n+1), \\ \lambda(m, n) = \frac{k}{c_v} \pi^2 \left[ \left( \frac{2m+1}{2L} \right)^2 + \left( \frac{2n+1}{w} \right)^2 \right], \quad (56)$$

where  $m$  and  $n$  take on values  $\{1, 2, 3, \dots\}$  and  $\{0, 1, 2, \dots\}$ , respectively.

The overlap integral for  $a_i$  can be evaluated as

$$o = \frac{-\sin \beta + \sinh \beta}{\cos \beta - \cosh \beta}, \quad \beta \\ = 4.730 \quad (\text{for first harmonic}), \\ \omega = \frac{\beta^2}{L^2} \sqrt{\frac{EI}{\rho A}} \quad (58)$$

and that the thermal modes are

$$\nu(m, n) = 2 \sin \pi \zeta m \sin \pi \eta (2n+1),$$

$$\lambda(m, n) = \frac{k}{c_v} \pi^2 \left[ \left( \frac{m}{L} \right)^2 + \left( \frac{2n+1}{w} \right)^2 \right], \quad (59)$$

the overlap integrals  $a_i$  can be found to be

$$a_i(m, n)_{\text{fixed-fixed}} = 2(3.4035) \left( \frac{2(-1)^n}{\pi^2(2n+1)^2} \right) \left( \frac{om\pi(-1)^{m+1} \cos(\beta) + m\pi(-1)^{m+1} \sin(\beta) + om\pi}{-\beta^2 + m^2\pi^2} \right) \\ + \frac{om\pi(-1)^{m+1} \cosh(\beta) + m\pi(-1)^{m+1} \sinh(\beta) + om\pi}{\beta^2 + m^2\pi^2}. \quad (60)$$

#### IV. DISCUSSION

The entropy generation based formulation offers three advantages over a fully coupled formulation. (1) The entropy generation is proportional to the sum of Lorentzians corresponding to individual thermal modes, thus providing insight into which thermal modes are responsible for the energy loss and an opportunity to mitigate the effect by suitably changing the thermal mode's frequency through design optimization. (2) The relatively simple formulation allows for estimation of a closed form expression for quality factor. (3) The entropy generation method naturally allows for estimation of entropy generated due to heat conduction in orthogonal directions, thus allowing an assessment of suitability of one-dimensional heat transfer assumption in resonator structure.

We first explore the sum of Lorentzian nature of the estimated quality factor and, in particular, the significance of the weighting coefficients  $b_i$ . Equation (25) bears a form similar to commonly established equation for finding the quality factor in a system with independent energy loss mechanisms

$$Q^{-1} = \sum_i Q_i^{-1}, \quad (61)$$

where  $Q_i$ 's are quality factors of independent energy loss mechanisms that contribute to the energy loss to their maximum potential. Thus the weighting factor  $b_i$  can be viewed as the potential of a thermal mode to cause energy loss. It is worthwhile to examine bounds of the weighting coefficients  $b_i$  in Eq. (25). Consider an extreme case when only one thermal mode contributes to the energy loss. This could happen, for instance, when the distribution of the heat generated due to the straining of the solid corresponds exactly with a single thermal mode. Then the summation in Eq. (25) would contain only one term, the modal Zener quality factor. It can be shown that for the cases of pure bending and uniaxial stress, the weighting factor  $b$  is identically equal to 1 (Appendix B). Thus we see that Zener's formula based on the assumption of single dominant thermal mode would still predict the quality factor accurately for the cases of pure bending and uniaxial stress. From the solution of the flexural resonators in Sec. III C, we find that a two-dimensional analysis reveals that the number of thermal modes with significant contribution to energy loss is, in fact, much greater than 1.

As seen from Sec. III, the entropic formulation enables calculation of closed form expressions for quality factor for several cases. The formulation also considerably reduces the time required to carry out numerical estimation of quality factor. For complex geometries, the thermal modes cannot be estimated analytically. However, by appropriate choice of approximate thermal modes, an approximate analytical estimation of quality factor can be carried out. It is also worth noting that the analytical formula presented for the fixed-fixed and the cantilever beams can be naturally extended to higher order mechanical modes by appropriate choice of value of mode dependent  $\beta$ , e.g.,

cantilever beam:

$$\beta_{\text{first flexural mode}} = 1.873,$$

$$\beta_{\text{second flexural mode}} = 4.652,$$

$$\beta_{\text{third flexural mode}} = 7.693,$$

fixed-fixed beam:

$$\beta_{\text{first flexural mode}} = 4.730,$$

$$\beta_{\text{second flexural mode}} = 7.662,$$

$$\beta_{\text{third flexural mode}} = 10.544. \quad (62)$$

Table I compares the quality factor of fixed-fixed beams possessing the same width but variable lengths vibrating in different mechanical modes. The quality factor of each mechanical mode is minimized when the resonant frequency is close to the dominant thermal mode frequency which is similar for all the vibrating modes.

We next consider the thermoelastic damping in bulk mode structures. Equation (29) asserts that in the limit of small values of the ratio of the frequency of thermal modes with large overlap with spatial distribution of volume change and mechanical mode frequency (i.e.,  $\lambda/\omega \ll 1$ ), the quality factor is inversely proportional to the frequency and independent of dimension of the resonator in any other way. A value of  $\psi$  can be estimated for flexural mode resonators which obey the same limit of  $\lambda/\omega \ll 1$  and this value is dependent on the dimensions of the flexural resonator unlike the case of bulk mode resonators. Next, we consider the significance of the constant  $\psi$  in Eq. (29). Large values of  $\psi$  result in higher

TABLE I. A comparison of quality factor of a fixed-fixed beam vibrating in different mechanical modes.

$w$ ( $\mu\text{m}$ )	$L$ ( $\mu\text{m}$ )	First mechanical mode		Second mechanical mode		Third mechanical mode	
		$f$ ( $10^6$ Hz)	$Q$ ( $10^4$ )	$f$ ( $10^6$ Hz)	$Q$ ( $10^4$ )	$f$ ( $10^6$ Hz)	$Q$ ( $10^4$ )
12	100	10.222	3.7971	26.821	8.7519	50.793	15.547
12	200	2.555	1.6279	6.705	3.7582	12.698	6.5722
12	300	1.136	1.0997	2.980	2.0713	5.643	3.5164
12	400	0.639	1.0944	1.676	1.4188	3.174	2.2227
12	500	0.409	1.3231	1.073	1.1829	2.031	1.6013
12	600	0.284	1.6964	0.745	1.1509	1.410	1.2967
12	700	0.209	2.1811	0.547	1.2380	1.036	1.1628
12	800	0.160	2.7627	0.419	1.4056	0.793	1.1319

energy loss due to thermoelastic dissipation. Table II summarizes the values for the constant  $\psi$  for silicon with Poisson’s ratio of 0.22 for various bulk mode structures. For fixed-fixed flexural beam of  $L/w$  ratio of 10, the constant  $\psi$  is of the order of  $10^4$ . Thus, in general, bulk modes exhibit much lower energy loss due to TED and the quality factor is inversely proportional to frequency up to gigahertz range of mechanical resonance frequencies. A notable extension to this rule is the case of extensional mode of a fixed-free beam whereby the quality factor has to be expressed as a sum over a large number of Lorentzians.

Finally, we examine the validity of one-dimensional analysis of TED in beams vibrating in flexural mode. The two-dimensional thermal modes take into account the fact that heat transfer occurs along the length of the beams as well as across the width. Heat transfer along any temperature gradient results in entropy generation. Thereby, heat transfer along the beam as well as across the beam must be taken into account. Thus, the limitation of the one-dimensional analysis can be explored by considering an entropy generation due to heat generation in the lateral direction. It can be seen that several thermal modes contribute significantly to the quality factor of a cantilever [Fig. 4(a)] and a fixed-fixed beam [Fig. 4(b)] resonator. Figures 5(a) and 5(b) show that inclusion of additional modes approaches the quality factor predicted by a finite element method based simulation. Furthermore, the Zener formula based prediction is also plotted in Fig. 5(b). Figures 6(a) and 6(b) show the percentage contribution of entropy generation due to heat transfer along the beam and the net entropy generated in the resonator over a period of vibration. It can be seen that the entropy generation due to heat transfer along the beam assumes significance (greater than 10% of the total entropy generation) for aspect ratios ( $L/w$ ) below 20. It should be noted that this aspect ratio is still greater than 10, above which Euler–Bernoulli beam as-

umption is valid. Zener’s formula, however, completely breaks down when the lateral heat transfer is much more significant. For instance, in a beam carrying a slot in the center, the entropy generated due to heat transfer along the beam is significant, as seen from Fig. 7. In these situations, it is required to find all the relevant overlap integrals and include all the thermal modes in the estimation of quality factor.

TABLE II. Values for constant  $\psi$  in Eq. (29) for various bulk mode resonator shapes and modes.

	Extensional mode	Lamé mode
Square	6.3	0
Ring	8.6	...
Disk	10	0.76

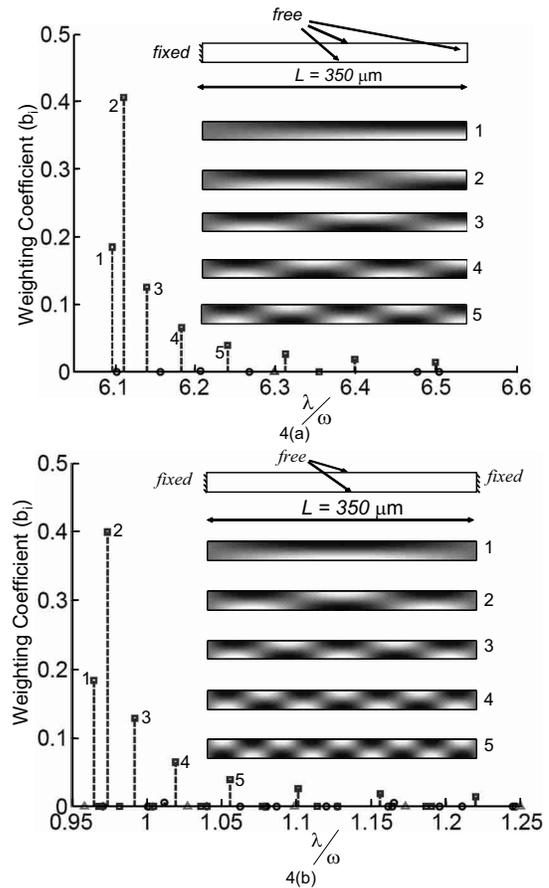


FIG. 4. Thermal mode contributions to lost work in (a) a cantilever and (b) a fixed-fixed beam. The inset shows a sample of significant thermal modes and their corresponding spatial distribution. The dark shaded regions correspond to temperatures higher than the reservoir temperature and the bright regions correspond to temperatures lower than the reservoir temperature.

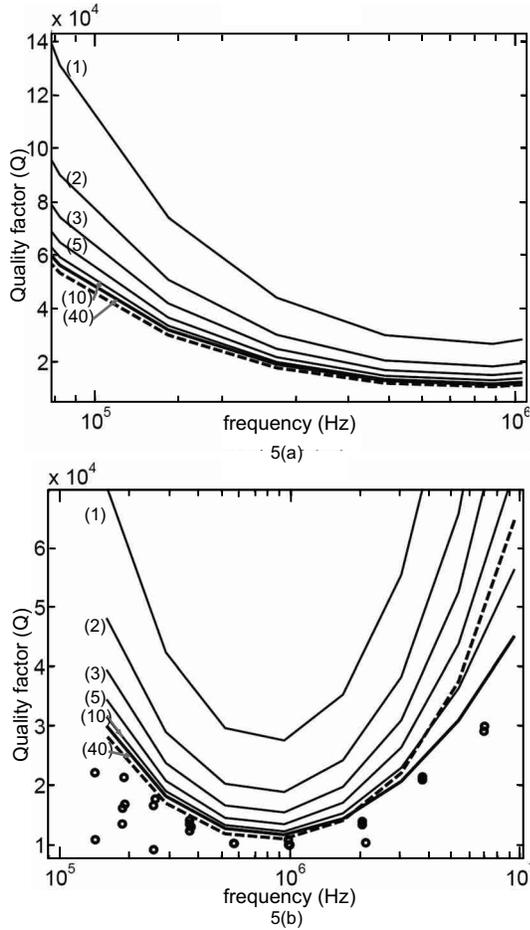


FIG. 5. Quality factor of (a) a cantilever and (b) a fixed-fixed beam. The dashed line corresponds to Zener formula based prediction. The solid lines depict the quality factor when the number of significant thermal modes contributing to the energy loss is equal to the number included next to the line. It can be seen that progressive inclusion of thermal modes finally converges to a value close to that predicted by Zener’s formula. The circular markers in Fig. 3(b) represent actual measured data.

**V. CONCLUSION**

In this paper we present an entropy generation based three-dimensional formulation of TED modeling in resonators. The quality factor estimated by using this modeling technique can be cast as a weighted sum of Lorentzians. We have obtained closed form expressions for quality factor limited by TED in different types of bulk mode, torsional, and flexural resonators by the application of the two-dimensional entropic formulation. We find that bulk mode resonators have much lower energy loss due to TED compared to flexural resonators. We also show that the two-dimensional formulation of flexural resonators reveals that several thermal modes contribute to the loss of energy in resonators unlike the one-dimensional analysis carried out by Zener. Approximate estimates of quality factor should be made by appropriate estimation of the weighting factor and judicious choice of thermal modes.

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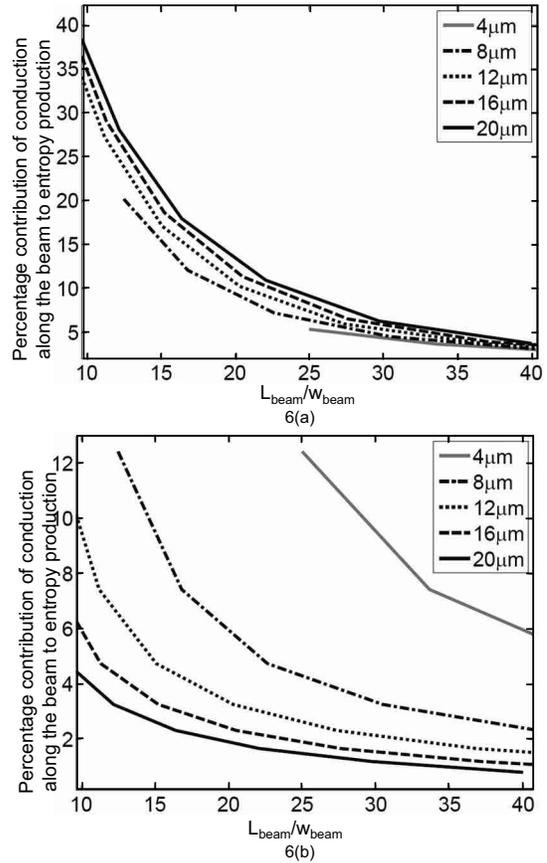


FIG. 6. Longitudinal heat transfer contribution to entropy generation in (a) cantilever and (b) fixed-fixed beam. The approximation of predominant heat transfer across the beam is worse in a fixed-fixed beam as compared to a cantilever. For  $L_{beam}/w_{beam}$  value of less than 20, the contribution of heat transfer along the beam is greater than 10% in the case of a fixed-fixed beam.

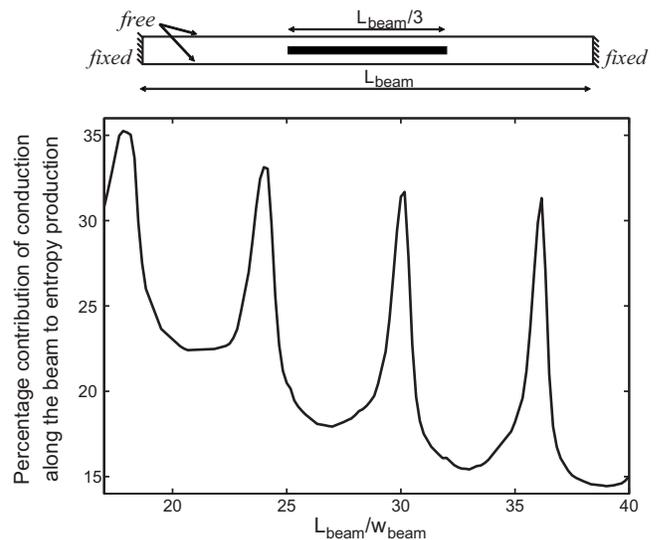


FIG. 7. Longitudinal heat transfer contribution to entropy generation in a fixed-fixed beam with a center slot as shown in the inset figure. In this case, there is significant contribution of lateral heat transfer as well as longitudinal heat transfer to entropy generation making it impractical to amend Zener’s formula to assess quality factor.

TABLE III. The weighting coefficient ( $b$ ) of a single dominant thermal mode for different strain constraints.

Strain constraint	Magnitude of weighting coefficient ( $b$ )	
	Arbitrary Poisson's ratio ( $\nu$ )	Silicon Poisson's ratio ( $\nu=0.2$ )
Isotropic strain	$\left(\frac{\partial u_1}{\partial x}\right) = \left(\frac{\partial u_2}{\partial y}\right) = \left(\frac{\partial u_3}{\partial z}\right)$ $\frac{3}{1-2\nu}$	5.1
Isotropic plane stress	$\left(\frac{\partial u_1}{\partial x}\right) = \left(\frac{\partial u_2}{\partial y}\right), \left(\frac{\partial u_3}{\partial z}\right) = -\frac{2\nu}{1-\nu}\left(\frac{\partial u_1}{\partial x}\right)$ $\frac{2}{1-\nu}$	2.5
Pure bending, uniaxial stress	$\left(\frac{\partial u_2}{\partial y}\right) = \left(\frac{\partial u_3}{\partial z}\right) = -\nu\left(\frac{\partial u_1}{\partial x}\right)$ 1	1

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## APPENDIX A: DERIVATION OF THERMOELASTIC HEAT EQUATION

We consider the change in temperature due to the change in volume of an adiabatic body.

$$\left(\frac{\partial T}{\partial V}\right)_S = -\frac{\left(\frac{\partial S}{\partial V}\right)_T}{\left(\frac{\partial S}{\partial T}\right)_V}. \quad (\text{A1})$$

Here,  $S$  is the entropy,  $T$  is the temperature, and  $V$  is the volume of the body in consideration. To estimate the ratio in Eq. (A1), we use the expression for entropy of a phonon gas.

$$S = k_B \sum_{\vec{k}s} \left\{ \frac{1}{k_B T} \frac{\hbar \omega_s(\vec{k}, V)}{e^{\hbar \omega_s(\vec{k}, V)/k_B T} - 1} - \ln[1 - e^{-\hbar \omega_s(\vec{k}, V)/k_B T}] \right\}, \quad (\text{A2})$$

$$\gamma_{\vec{k}s} = -\frac{V}{\omega_s(\vec{k}, V)} \frac{\partial \omega_s(\vec{k}, V)}{\partial V}, \quad (\text{A3})$$

where  $\vec{k}$  is the wavenumber of phonon mode,  $s$  is the polarization of phonon mode,  $\omega_s(\vec{k})$  is the phonon mode frequency corresponding to wavenumber  $\vec{k}$ , and  $\gamma_{\vec{k}s}$  is modal Grüneisen's parameter.

Thus, evaluating the required terms for Eq. (A1) as

$$\left(\frac{\partial S}{\partial V}\right)_T = \sum_{\vec{k}s} \frac{[\hbar \omega_s(\vec{k}, V)]^2 \gamma_{\vec{k}s}}{k_B T^2} \frac{e^{\hbar \omega_s(\vec{k}, V)/k_B T}}{V [e^{\hbar \omega_s(\vec{k}, V)/k_B T} - 1]^2} = \gamma_{c_v} \quad (\text{A4})$$

and

$$\left(\frac{\partial S}{\partial T}\right)_V = \sum_{\vec{k}s} \frac{[\hbar \omega_s(\vec{k}, V)]^2}{k_B T^3} \frac{e^{\hbar \omega_s(\vec{k}, V)/k_B T}}{[e^{\hbar \omega_s(\vec{k}, V)/k_B T} - 1]^2} = \frac{c_v}{T}, \quad (\text{A5})$$

we obtain an expression for change in temperature due to change in volume at constant entropy.

$$\left(\frac{\partial T}{\partial V}\right)_S = -\frac{T}{V} \gamma. \quad (\text{A6})$$

Equation (A6) can be used to obtain a heat source term in the heat equation. We use the differential form for change in temperature

$$dT = \left(\frac{\partial T}{\partial S}\right)_V dS + \left(\frac{\partial T}{\partial V}\right)_S dV. \quad (\text{A7})$$

The rate of change in entropy in a body while neglecting the entropy production can be found by combining the second law of thermodynamics with Fourier's law of heat transfer.

$$\frac{dS}{dt} = \frac{1}{T} \frac{\partial Q}{\partial t} = \frac{k \nabla^2 T}{T}. \quad (\text{A8})$$

The rate change in volume of a body can be expressed in terms of the rate change in principal strains  $\dot{\epsilon}_1$ ,  $\dot{\epsilon}_2$ , and  $\dot{\epsilon}_3$  in the body.

$$\left[\frac{\partial}{\partial t} \left(\frac{\delta V}{V}\right)\right] = \dot{\epsilon}_1 + \dot{\epsilon}_2 + \dot{\epsilon}_3. \quad (\text{A9})$$

Substituting Eqs. (A8) and (A9) into Eq. (A7), one obtains the heat equation with a heat source term that depends on the rate of change in volume.

$$c_v \frac{\partial T}{\partial t} = k \nabla^2 T - \gamma_{c_v} T \left[ \frac{\partial}{\partial t} \left(\frac{\delta V}{V}\right) \right] = k \nabla^2 T - \gamma_{c_v} T (\dot{\epsilon}_1 + \dot{\epsilon}_2 + \dot{\epsilon}_3). \quad (\text{A10})$$

## APPENDIX B: WEIGHTING COEFFICIENT FOR A SINGLE MODE THERMOELASTIC DAMPING CASE FOR SPECIAL STRESS-STRAIN CONDITIONS

It will be shown that under specific strain conditions, the proportionality constant  $\phi$  can be evaluated exactly. Consider the case of pure bending wherein the principal strains approximately satisfy the relationship

$$\left(\frac{\partial u_2}{\partial y}\right) = \left(\frac{\partial u_3}{\partial z}\right) = -\nu \left(\frac{\partial u_1}{\partial x}\right). \quad (\text{B1})$$

Substituting Eq. (B1) in the strain normalizing condition given by Eq. (15), we obtain

$$\int_V \left(\frac{\partial u_1}{\partial x}\right)^2 = \frac{1}{(1-2\nu)^2}. \quad (\text{B2})$$

Upon substitution of Eqs. (B1) and (B2) into Eq. (24),

$$\phi = \frac{1}{2(1-2\nu)^2}. \quad (\text{B3})$$

If a single thermal mode completely overlaps exactly with the volume change distribution in the solid, in the case of pure bending, the weighting coefficient  $b$  of that mode can be shown to be equal to 1 by substituting Eq. (B3) into Eq. (25). Table III shows some other common strain constraints and the resulting magnitude of weighting coefficient ( $b$ ) of the single active thermal mode.

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