LIMITS OF QUALITY FACTOR IN BULK-MODE MICROMECHANICAL RESONATORS

S. A. Chandorkar[1], M. Agarwal[1], R. Melamud[1], R. N. Candler[1], K. E. Goodson[1] and T. W. Kenny[1]
[1] Departments of Electrical & Mechanical Engineering, Stanford University

ABSTRACT

In this paper we present the dominant energy loss mechanisms and quality factor (Q) limits in bulk mode micromechanical resonators. We demonstrate that in resonators with an appropriately designed stem connection to anchor the maximum achievable Q limit is set by either Thermoelastic dissipation (TED) or the Akhieser effect (AKE). Furthermore, we suggest a choice of materials for achieving maximum Q's in micromechanical resonators. It is established here that silicon resonators can theoretically achieve higher Q's than quartz and we predict that by using alternative materials, such as silicon carbide, it is possible to surpass the Q of quartz by more than an order of magnitude.

1. INTRODUCTION

Micromechanical resonators have the potential to replace quartz crystals for timing and frequency references owing to their small form factors, CMOS integrability, low cost, and low power operation [1]. Resonators with good frequency stability and high quality factors (Q) are critical for high performance reference oscillators [2].

Micromechanical resonator designs can be broadly classified as per their mode of operation namely flexural, torsional and bulk mode devices (Fig. 1a). Flexural vibration modes can be viewed as transverse standing waves. In the flexural devices, the displacement of the structures is orthogonal to the bending stress in the structure. In torsional resonators, the dominant stress is shear stress and the displacement is rotational. Bulk mode operation of resonators is representative of standing longitudinal waves. Fig. 1b shows the commonly used bulk-mode device designs shapes such as circular disk and square plate that may be operated in Lamé, wine-glass and extensional (contour) modes.

In this paper, we will examine the Q limits of some of the bulk mode structures. Q is a measure of energy loss in a resonator and is defined as

$$Q = 2\pi \frac{U_{max-stored}}{W_{lost}} \tag{1}$$

where, $U_{max\text{-}stored}$ is maximum energy stored and W_{lost} is the energy lost during an oscillation cycle. The commonly encountered energy loss mechanisms in micromechanical resonators are air damping, Thermoelastic dissipation (TED), resistive damping and clamping loss. Fig. 2 depicts the frequency dependence of some of these energy loss mechanisms. Air damping, being inversely proportional to resonant frequency [3], is the dominant energy loss mechanism at low frequencies. TED has been studied extensively for flexural devices [4,5] and exhibits Lorentzian type of frequency dependence.

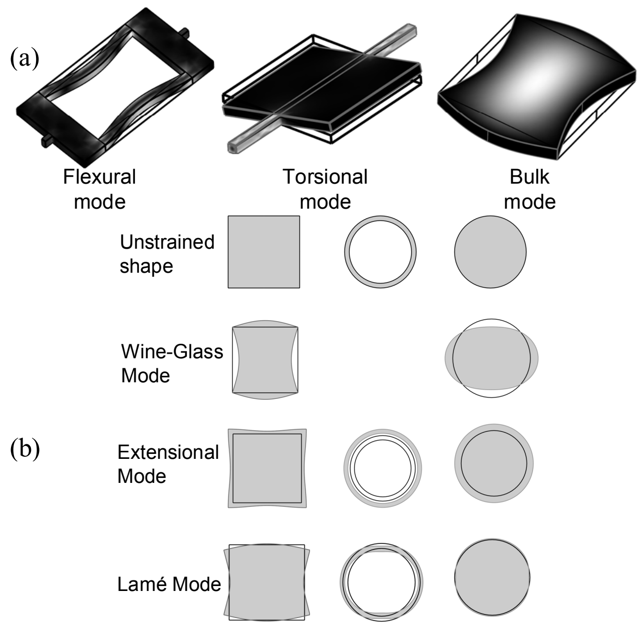

Figure 1: (a)Three basic types of resonators: Flexural, Torsional and Bulk mode structures (b) Commonly used Bulk mode resonator designs and various mode shapes

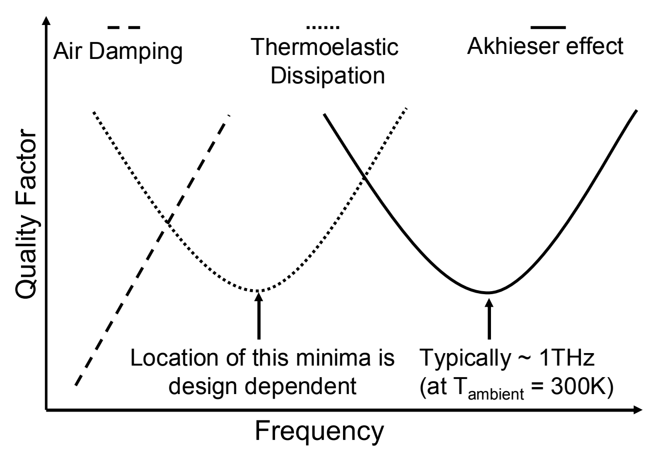

Figure 2: Energy loss mechanisms and their dependence on frequency: a) Air Damping b) Thermoelastic Dissipation in flexural structures c) Akhieser effect.

The dominant energy loss mechanism in bulk mode devices, typically being high frequency devices, is considered to be clamping loss. Clamping loss is design dependent and at any given frequency this loss can be dominant energy loss mechanism if the stem connecting the resonator to the anchor is inappropriately designed [6-9].

Through this work, we will be show that TED limits the Q for Lamé mode devices. We introduce an energy loss mechanism called Akhieser effect (AKE), which imposes a

Q limit on high frequency devices if TED is minimized, as is the case with wine glass mode and contour mode.

2. THEORY

We consider a small control volume in a vibrating solid. The phonon dispersion in the control volume is perturbed due to strain which in turn results in non-equilibrium of phonon population. Equilibrium can be reestablished in the solid by normal and Ümklapp processes of relaxation and by flow of phonons in and out of the control volume under consideration. The Boltzmann transport equation (BTE) captures these phonon dynamics [10, 11]. Attainment of equilibrium from this non-equilibrium state will result in entropy generation if this relaxation is not in phase with the vibration rate. If the equilibrium is established purely by normal and Ümklapp processes, (i.e. the process is purely local) the resulting energy loss is AKE. On the other hand, if the equilibrium of phonon population is largely established due to flow of phonons from beyond the control volume in question, the resulting energy loss is TED. Fig. 3 schematically depicts the essential differences between AKE and TED. In this section, we seek to quantify TED and AKE.

2.1 Thermoelastic dissipation

In order to quantify TED, we introduce the concept of thermal modes [4]. Thermal modes are eigenmodes of the homogeneous heat diffusion equation. The temperature distribution of the resonator can be expressed as a weighted sum of these thermal modes. The magnitude of these weights depends on overlap of the spatial distribution of thermal mode with the strain distribution and is given by

$$a_i \propto \frac{\int_V \nabla \cdot \bar{U}(x,y,z) v_i(x,y,z) d\Omega}{\int_V v_i^2(x,y,z) d\Omega} \tag{2}$$

where, a_i is weight of the thermal mode v_i and $\bar{U}$ is the strain in the solid. The greater the weighting factor of a thermal mode, the greater is its contribution to entropy generation ($\Delta S_{generation}$).

$$\Delta S_{generation} \propto \frac{\alpha^2 B^2}{c_v} \sum_i a_i^2 \frac{f\lambda_i}{f^2 + \lambda_i^2} \tag{3}$$

where, f and λ are mechanical resonance frequency and thermal mode eigenfrequency respectively. Energy lost in a resonator is directly proportional to the entropy generation and the ambient temperature.

$$W_{lost} = T_{amb} \Delta S_{generation} \tag{4}$$

where, T_{amb} is the ambient temperature. TED is minimized if the overlap integral in (2) is minimized or if the lorentzian is minimized.

The high stiffness of bulk mode devices ensures that for high frequency structures the λ is typically much smaller than f. Thus,

$$W_{lost,bulk} \propto \frac{\alpha^2 B^2}{c_v} \sum_i a_i^2 \frac{\lambda_i}{f} \tag{5}$$

where, α is the coefficient of thermal expansion, B is the

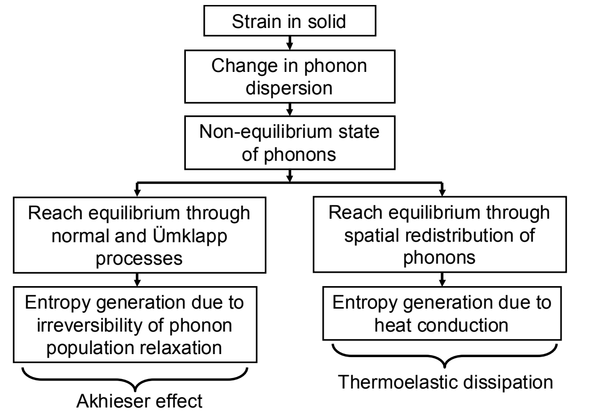

Figure 3. Schematic of Akhieser effect and Thermoelastic dissipation.

bulk modulus and c_v is the heat capacity per unit volume. Furthermore, λ is given by

$$\lambda_i \propto \frac{k_{thermal}}{c_v} \frac{1}{L^2} \left(2(2i+1)^2\right) \tag{6}$$

where, $k_{thermal}$ is the thermal conductivity and L is a characteristic length scale of the bulk mode resonators. The resonant frequency f of bulk mode structures is given by

$$f \propto \frac{1}{L} \sqrt{\frac{E}{\rho}} \tag{7}$$

where, E is the elastic modulus and ρ is the density of the structure. Substituting (6) and (7) in (5) and noting that the $U_{max\text{-}stored}$ is proportional to E, we obtain, after appropriate mathematical manipulation of the resulting expression, an expression for $Q_{TED,Bulk}$ in terms of its mechanical resonant frequency.

$$Q_{TED,Bulk} = \frac{1}{\psi} \frac{c_v^2}{\alpha^2 \rho k_{thermal} T} \frac{1}{f} \tag{8}$$

This expression, though quite general, does depend on the specific design of the bulk mode structure through the constant ψ. Next, we introduce another thermo-mechanical loss that is entirely local in its nature, and thereby, independent of the precise geometry of the structure.

2.2 Akhieser effect

Owing to local nature of AKE, any given control volume in a vibrating structure undergoes periodic strain with no interaction with its surrounding as far as attainment of equilibrium of phonon populations is concerned. Thus, a result for measure of energy loss due to AKE from the field of acoustics will be valid for resonators as well. In this paper, we quote the result from [10] which examines AKE in solids subject to ultrasonic vibrations

$$\Gamma = \frac{fW_{lost}}{ce_{stored}} = \frac{4\pi^2 f^2 \gamma^2 T_{amb} k_{thermal}}{\rho c^5} \tag{9}$$

where, e_{stored} is energy stored per unit volume, γ is Grüneisen's parameter and c is acoustic velocity. The energy stored per unit volume is given by

$$e_{stored} = \frac{1}{2}\rho(2\pi f)^2\left(u_1^2 + u_2^2 + u_3^2\right) \tag{10}$$

where, u_i is the displacement along i^{th} orthogonal direction.

Substituting (10) in (9) and recalling the definition of Q from (1),

$$Q_{AKE} = \frac{\rho c^2}{2\pi\gamma^2 c_v T}\frac{1}{f} \quad (11)$$

It should be noted that (11) carries no additional information about the exact geometry of the structure other than the resonant frequency. Thus, if Q of a device is AKE limited, the *Q-f* product of the device is solely dependent on material properties.

In the following section, we will consider specific geometries of bulk mode structures shown in Fig. 1b and investigate the material property limit of quality factor for each.

3. CASE STUDIES AND EXPERIMENTAL EVIDENCE

In this section, we will consider three major modes of operation in bulk mode devices and estimate the limit of Q for these structures.

3.1 Lamé mode

Structures operated in Lamé mode have regions of compression and tension, thereby, making them susceptible to energy loss due to TED. However, since the λ of thermal modes that have significant overlap with strain pattern is much lesser than f, (8) is applicable for Q estimation of Lamé modes. Table 1 lists the factor ψ for the two geometries with Lamé mode shown in Fig. 1b. Fig. 4 shows the mechanical mode and corresponding first three thermal modes. The AKE estimate of Q for these structures is of the same order as TED. Following the discussion in section 2, TED is likely to set the lower limit of energy loss in Lamé modes if the estimates from the formulae (8) and (11) are comparable.

3.2 Wine glass mode

Wine glass mode of a square resonator has a unique strain pattern in that it is inherently isochoric. Fig. 5a shows the principle strain pattern in the wine glass mode. Therefore, as per (2), the primary driving force of TED is absent. This mode in square resonators is limited by AKE. Though the deformation is not perfectly isochoric in disk resonators, as the structure is not limited by TED to the first order, upper limit of Q is still set by AKE.

3.3 Extensional mode

Fig. 5b shows the distribution of volumetric change in an extensional mode of a ring. It can be seen that, extensional mode structures have large "dc" offset of volumetric strain. From the formulation of entropy production due to TED (3), the a_i for the "dc" thermal mode is high. To the first order extensional mode devices do not suffer from TED losses. Thus, Q limit of this mode is also set by AKE.

Table 2 lists estimated Q limits for a square resonator in various modes. We see that upper limit of Q in Lamé mode of this resonator will be TED limited while in wine-glass mode and extensional mode it is AKE limited.

Shape	ψ
Square	$25(1+\upsilon)$
Disk	$5.1(1+\upsilon)$

Table 1: ψ estimated for Lamé modes (υ: Poisson ration)

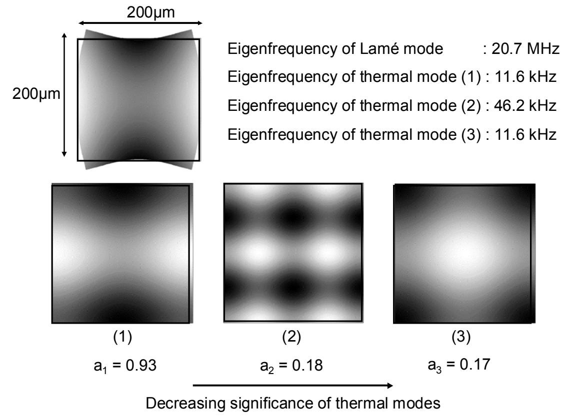

Figure 4: TED in Lamé mode of square resonator (a) Mechanical mode (b) First three thermal modes

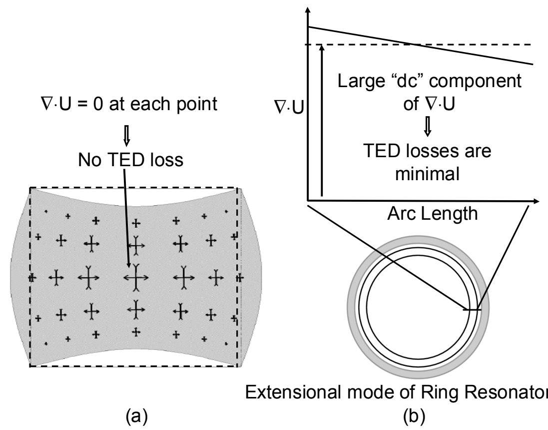

Figure 5: TED in (a) wine glass mode of a square resonator (b) extensional mode of a ring resonator

	Lamé	Wine-glass	Extensional
TED	5.8×10^6	$\sim10^{10}$	19.1×10^6
AKE	2×10^6	2.1×10^6	1.9×10^6

Table 2: Estimated Q of a square resonator with edge length of 200µm

Fig. 6 compares some of the state of the art devices against the Q upper limits imposed by TED and AKE on single crystal devices. The marked forbidden zone is for single crystal silicon based micromechanical resonators.

4. DISCUSSION

We first make a note of surprising similitude of the formulae for TED and AKE in spite of the difference in the nature of the two effects as discussed in the theory section. This can be reconciled to some extent by noting that the initial cause of the non-equilibrium is the same and if both the effects are equally efficient in carrying the system toward equilibrium, the entropy generation would be similar.

Another striking aspect of the two effects is that the *Q-f*

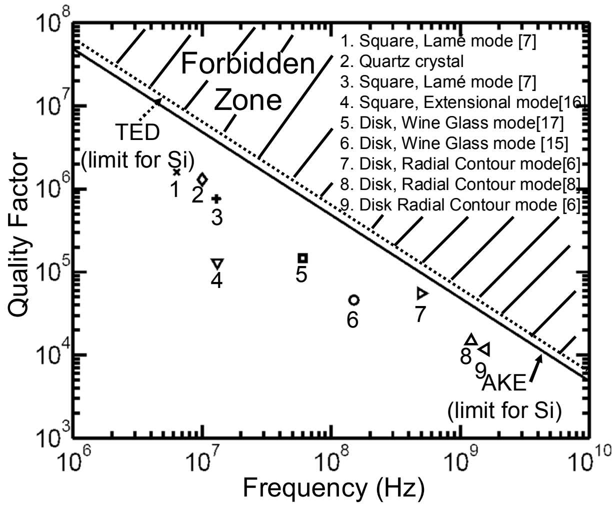

Figure 6: Quality factor and frequency products of recently reported high frequency devices.

Material	*Q-f* (x 10^{13})	γ
Si	3.9	0.51
Quartz	3.2	0.87
AlN	2.5	0.91
Diamond	3.7	0.94
Sapphire	11.3	1.1
SiC	64	0.3

Table 3. Akhiezer effect limit of Q-f product for resonators composed of different materials

products are constant for a given material and mode shape. Table 3 lists some of the commonly used resonator materials and their *Q-f* products together with the Grüneisen parameter used to determine these limits. It is evident that SiC has exceptionally high *Q-f* product.

It should be noted that the quality factor limits mentioned here represent maximum achievable quality factor for a device. Thus, a measure of goodness of design of the clamping structure is the difference between the actually measured quality factor and the ascribed limits. Figure 6 shows that one of the most efficient designs for reducing clamping loss was achieved by a composite ring structure [12].

At this point, it is necessary to point out that the limits calculated in this paper have been based off of material properties data found from literature. However, these values are generic and for the specific device exact knowledge of these properties is required. Among others, the most difficult value to ascertain is the Grüneisen parameter.

5. CONCLUSION

In this paper, we have analyzed the quality factor limits of bulk mode devices. We show that for bulk mode structures, TED assumes a form such that *Q* is inversely proportional to *f*. We introduce a relatively unknown loss mechanism in context of micromechanical resonators called Akhieser effect. We show that Akhieser effect is independent of the geometry of the structure and the resulting *Q-f* product is purely material property limited. Quality factor limit of Lamé mode of structures is determined by TED while that of extensional and wine glass modes is AKE limited. Finally, we show that Si has a *Q-f* product which is marginally greater than quartz and a ~20x higher *Q-f* product can be achieved by using SiC.

6. ACKNOWLEDGEMENTS

This work was supported by DARPA HERMIT (ONR N66001-03-1-8942), Bosch Research and Technology Center (RTC) and the National Nanofabrication Users Network facilities funded by the National Science Foundation under award ECS-9731294, and The National Science Foundation Instrumentation for Materials Research Program (DMR 9504099). The authors wish to thank Dr. Amy Duwel from Draper Labs for useful discussions.

7. REFERENCES

[1]C. T. C. Nguyen, "*MEMS for Frequency Control and Timing*", presented at IEEE FCS, 2005.

[2]C. T.-C. Nguyen, "*Vibrating RF MEMS technology: fuel for an integrated micromechanical circuit revolution*", presented at Transducers, 2005.

[3]J. Wang et al., "*1.156GHz Self-aligned vibrating micromechanical disk resonator*", IEEE transactions on Ultrasonics, Ferroelectrics and Frequency Control, 2004.

[4]A. Duwel et. al., "*Engineering MEMS Resonators with LOW Thermoelastic Damping*", IEEE Journal of Microelectromechanical Systems, 2006.

[5] R. N. Candler et Al., "*Investigation of Energy Loss Mechanisms in Micromechanical Resonators*", Transducers 2003.

[6]J. Wang et al., "*1.51-GHz polydiamond micromechanical disk resonator with impedance-mismatched isolating support*", MEMS 2004.

[7]Khine et.al., "*6MHz bulk-mode resonator with Q values exceeding one million*", Transducers, 2007.

[8]Sheng-Shian et al., "*Micromechanical hollow-disk ring resonators*", MEMS 2004.

[9]Siavash Pourkamali et al."*VHF Single Crystal Silicon Capacitive Elliptic Bulk-Mode Disk Resonators*", JMEMS 2004.

[10]Woodruff et al., "*Absorption of Sound in Insulators*", Phys. rev. 1961

[11]H. H. Barrett et al., "*Critique of Current Theories of Akhieser Damping in Solids*", Phys rev. 1970

[12]J.Wang et al.,"*1.51-GHz polydiamond micromechanical disk resonator with impedance-mismatched isolating support*", MEMS 2004.

[13]Khine et.al., "*6MHz bulk-mode resonator with Q values exceeding one million*", Transducers, 2007.

[14]Sheng-Shian et al., "*Micromechanical hollow-disk ring resonators*", MEMS 2004.

[15]Siavash Pourkamali et al."*VHF Single Crystal Silicon Capacitive Elliptic Bulk-Mode Disk Resonators*", JMEMS 2004.

[16] Kazaakari et al., "*Square extensional mode single - crystal silicon micromechanical resonator for low phase noise oscillator applications*", IEEE Electron Device Letter., April 2004.

[17] Y.W Lin et al., "*Series-resonant VHF micromechanical resonator reference oscillators*", ISSC 2004.