

EFFECT OF PHONON INTERACTIONS ON LIMITING THE $f.Q$ PRODUCT OF MICROMECHANICAL RESONATORS

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ABSTRACT

We discuss the contribution of phonon interactions in determining the upper limit of $f.Q$ product in micromechanical resonators. There is a perception in the MEMS community that the maximum $f.Q$ product of a microresonator is limited to a “frequency-independent constant” determined by the material properties of the resonator [1]. In this paper, we discuss that for frequencies higher than $\omega_\tau = 1/\tau$, where τ is the phonon relaxation time, the $f.Q$ product is no longer constant but a linear function of frequency. This makes it possible to reach very high Q s in GHz micromechanical resonators. Moreover, we show that $\langle 100 \rangle$ is the preferred crystalline orientation for obtaining very high Q in bulk-acoustic-mode silicon resonators above ~ 750 MHz, while $\langle 110 \rangle$ is the preferred direction for achieving high- Q at lower frequencies.

KEYWORDS

Akheiser regime, attenuation coefficient, phonon interaction, Landau-Rumer regime, resonator, $f.Q$ product, Q , ultrasonic absorption.

INTRODUCTION

Several dissipative mechanisms limit the Q of an electromechanical resonator [1], [2], [3]. Among those, some can be suppressed and even eliminated through proper design (e.g. clamping loss [3]). However, some energy dissipation mechanisms are intrinsic to the resonating material. The “intrinsic Q ” of a resonator is defined as

$$Q = 2\pi \frac{\text{Energy stored}}{\text{Energy dissipated per cycle of oscillation}}. \quad (1)$$

For an acoustic wave propagating in solids, the sound abortion coefficient, $\alpha(\omega)$, defined as [4]

$$\alpha(\omega) = \frac{1}{2} \frac{\text{Mean energy dissipated}}{\text{Energy flux in the wave}} \quad (2)$$

is a measurable quantity and describes the variation in the wave amplitude with propagation distance. Therefore, by definition Q and $\alpha(\omega)$ are related through

$$Q = \frac{\omega}{2\alpha(\omega)V_a}, \quad (3)$$

where V_a is the wave velocity and ω is the angular resonance frequency.

A figure of merit for micromechanical resonators is the $f.Q$ product. Using (3), we have

$$\omega f.Q = \frac{\omega^2}{2\alpha(\omega)V_a}. \quad (4)$$

The fundamental intrinsic dissipation mechanisms limiting the $f.Q$ product of resonators consist of thermoelastic, phonon-electron, and phonon-phonon interactions (see Table 1). Among these, the phonon-phonon dissipation is the dominant intrinsic loss mechanism in semiconducting and insulating resonators at room temperature. In this paper, we focus on the phonon-phonon dissipations and show that at room temperature, $f.Q$ of a micromechanical resonator due to this intrinsic dissipation mechanism is frequency dependent.

DISSIPATION DUE TO PHONON-PHONON INTERACTIONS

Two different approaches have been taken to describe the physics of ultrasonic attenuation due to the interaction of an acoustic wave with thermal phonons:

(a) In the approach that was first introduced by Akheiser [5], the sound wave is regarded as a macroscopic strain field in the crystal. Since the frequency of thermal phonons depends on the strain, the thermal equilibrium is disturbed [2], leading to ballistic transport of phonons between hot and cold regions (as opposed to the diffusive transport of heat in the thermoelastic dissipation). The process of restoring the thermal equilibrium to the phonon gas is accompanied by dissipation of energy from the acoustic wave. The response of the phonon system to the acoustic wave is calculated by means of the phonon Boltzmann equation [6].

(b) An alternative approach was given by Landau and Rumer [7]. Here, the acoustic wave is regarded as a parallel beam of low-energy phonons. Because of anharmonic terms in the Hamiltonian of the crystal, interactions between different modes are possible and the rate at which the acoustic phonons are scattered is calculated by the perturbation theory [8].

Both approaches are valid based on some assumptions on wavelength of the propagating acoustic wave as well as the life time of thermal phonons (which depends on the temperature of the acoustic material). In this paper, we focus on the nature of the acoustic attenuation *at room temperature* (300 °K) and only consider the frequency dependency of the phonon-phonon dissipations.

Table 1. Simplified expressions for $\alpha(\omega)$ and $f \cdot Q$ (ω : acoustic angular frequency, ρ : density, V_a : acoustic velocity, κ : thermal conductivity, β : thermal expansion coefficient, σ : electrical conductivity, m_e : electron mass, ε_F : Fermi energy, e : electron charge, C_v : volumetric heat capacity, T : absolute temperature, γ : Grüneisen parameter, h : Planck constant, and K : Boltzmann constant).

	Thermoelastic Dissipation	Phonon-electron Dissipation	Phonon-phonon Dissipation
α	$\alpha = \frac{\kappa T \beta^2 \rho \omega^2}{18 V_a^3} \quad \omega \tau^* < 1 [2]$	$\alpha = \frac{4 \varepsilon_F m_e \sigma}{15 \rho e^2 V_a^3} \omega^2 [2]$	$\begin{cases} \alpha(\omega) = \frac{C_v T \gamma^2 \tau}{2 \rho V_a^3 (1 + (\omega \tau)^2)} \omega^2 & \omega \tau < 1 [2] \\ \alpha(\omega) = \frac{\pi^5 \gamma^2 K^4 T^4}{30 \rho V_a^6 h^3} \omega & \omega \tau > 1 [7] \end{cases}$
$f \cdot Q$	$f \cdot Q_{TED} = \frac{9 V_a^2}{\kappa T \beta^2 \rho} \cdot 2\pi i$	$f \cdot Q_{phe} = \frac{15 \rho e^2 V_a^2}{8 \varepsilon_F m_e \sigma} \cdot 2\pi i$	$\begin{cases} f \cdot Q_{PhP} = \frac{\rho V_a^2 (1 + (\omega \tau)^2)}{C_v T \gamma^2 \tau} \cdot 2\pi i & \omega \tau < 1 \\ f \cdot Q_{PhP} = \frac{15 \rho V_a^5 h^3}{\pi^5 \gamma^2 K^4 T^4} \omega & \omega \tau > 1 \end{cases}$
Remarks	Negligible in semiconductor with proper design. Dominant intrinsic source of loss in metals.	Negligible in insulators and doping dependent in semiconductors at room temperature.	Dominant intrinsic loss in semiconductors and insulators.

Akheiser Regime

If the acoustic wavelength (λ) is considerably larger than the mean free path of phonons ($\omega \ll 1/\tau$), we can assume that the acoustic wave is interacting with the whole ensemble of thermal phonons. Therefore, *locally* changing the phonon frequencies and perturbing the phonon distribution function away from its equilibrium Planck form. This range ($\omega \ll 1/\tau$) is known as the Akheiser regime.

In Akheiser regime, the wave equation can be formulated based on the modified Hooke's law, proposed by Zener [9], and the second law of Newton as follows:

$$c_R \cdot \frac{\partial^2 V}{\partial z^2} + \eta \cdot \frac{\partial^3 V}{\partial t \cdot \partial z^2} - \frac{\eta}{c_U} \cdot \rho \cdot \frac{\partial^3 V}{\partial t^3} = \rho \cdot \frac{\partial^2 V}{\partial t^2}, \quad (5)$$

where c_R and c_U are the relaxed and un-relaxed elastic stiffness constants, η is the *effective* viscosity of the acoustic material, and V is the velocity. Assuming a plane wave solution $V = e^{j(\omega t - kz)}$ and considering the acoustic absorption, we have: $k = \chi - j\alpha(\omega)$. In all practical cases $\alpha(\omega)$ is very small compared to χ and ω [10]. Therefore:

$$\frac{\omega}{\chi} = \sqrt{\frac{c_R}{\rho}} = V_a, \quad (6)$$

$$\alpha(\omega) = \frac{\omega^2 \cdot \eta \cdot (c_U - c_R)}{2 \cdot V_a \cdot c_U \cdot c_R} \quad (7)$$

For *longitudinal* acoustic waves in Akheiser regime, the acoustic attenuation is proportional to ω^2 , hence the

$f \cdot Q_{PhP}$ product is constant (see Eq. 4). For *transverse* waves in the Akheiser range, $\alpha(\omega)$ is theoretically proportional to $\omega^{1.75}$ [11]. Therefore, $f \cdot Q_{PhP}$ has a slight frequency dependency ($f \cdot Q_{PhP} \propto \omega^{0.25}$). A dependence of this kind has been observed in many crystals [11], and may be due to the presence of impurities, which heavily influences the attenuation in transverse acoustic wave but may only slightly affect the longitudinal waves [12].

Landau-Rumer Regime

When λ is less than the phonon mean free path, the acoustic quanta interact with individual lattice phonons. In the Landau-Rumer regime ($1/\tau \ll \omega \ll KT/h$), acoustic attenuation is mainly due to three-phonon interactions and can be shown to be linearly proportional to ω (Table 1) [7]. Therefore, the $f \cdot Q$ product will not be constant but *increases linearly* with ω (Table 1).

Landau-Rumer Effect at Room Temperature

The transition from Akheiser to Landau-Rumer regime occurs at $\omega_\tau = 1/\tau$, which can be estimated as

$$\omega_\tau = \frac{C_v V_D^2}{3n\kappa} \left(\frac{3}{V_D^3} = \frac{1}{V_l^3} + \frac{2}{V_t^3} \right), \quad (8)$$

where V_D , V_l , and V_t are the mean Debye, longitudinal and transverse velocities, respectively. We define n as a correction factor, which is close to 1 for transverse waves. The reason for this is that for transverse sound waves τ is usually assumed to be close to the thermal relaxation time τ_C . For longitudinal waves, the direct interaction with

thermal phonons is forbidden and therefore, τ becomes greater (n is close to 2).

The condition of $\omega \gg 1/\tau$ is easier met at low temperatures as τ increases rapidly with falling temperature [12]. At room temperature, for most semiconductors, ω_τ occurs in the GHz range (1-20 GHz) [13]. Interestingly, for acoustic wave propagating in $\langle 100 \rangle$ orientation of silicon, τ is an order of magnitude larger than that of the other directions. This has been experimentally verified in [12], where the value of τ was extracted from the kink in the measured frequency-dependent acoustic attenuation curve. The significance of this effect is pronounced at frequencies above $\omega_\tau = 2\pi f_\tau = 1/\tau$, where $f \cdot Q_{PhP}$ increases with frequency (Fig. 1). For silicon in $\langle 100 \rangle$ direction, f_τ is ~ 700 MHz.

To understand the reason for relatively large phonon relaxation time of longitudinal waves propagating in $\langle 100 \rangle$ direction in silicon, one has to consider the anharmonic phonon decay model of Landau and Rumer to account for only the types of phonon collisions that are allowed by the crystalline anisotropy [4], [14]. In $\langle 100 \rangle$ direction in silicon, out of all allowed interactions, only those with transverse phonons contribute to absorption (or acoustic attenuation). The absorption of the longitudinal acoustic wave in $\langle 110 \rangle$ direction, on the other hand, is governed by its interaction with longitudinal thermal phonons only [12]. Hence, the relaxation time of thermal phonons depends on its interaction with transverse phonons in $\langle 100 \rangle$ direction, and with longitudinal phonons in $\langle 110 \rangle$ direction. The life time of transverse thermal phonons decreases less rapidly with increasing temperature (Fig. 2). Therefore, at room temperature, τ in $\langle 100 \rangle$ direction in silicon remains larger, while in other direction, τ is decreased significantly.

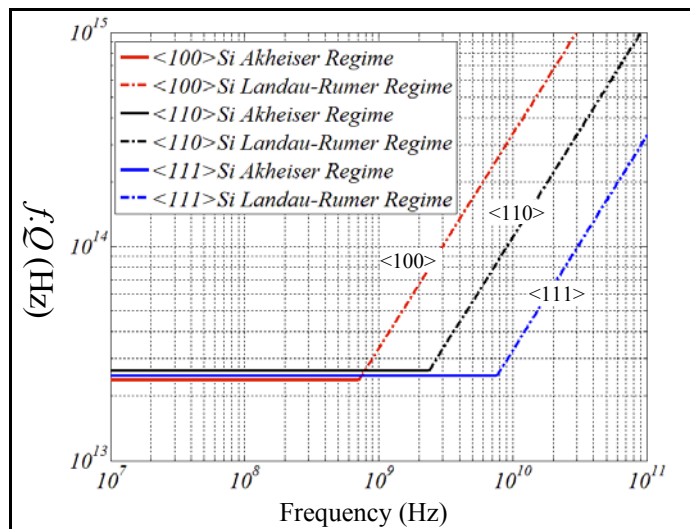


Figure 1. Comparison of $f \cdot Q_{PhP}$ for acoustic wave propagating in different crystallographic directions in silicon. The value of ω_τ ($\omega_\tau = 1/\tau$) is extracted from the data for τ presented in [15].

To demonstrate the significance of phonon-phonon interactions on limiting the $f \cdot Q$ of a semiconducting or insulating micromechanical resonator, the $f \cdot Q_{PhP}$ of $\langle 100 \rangle$ silicon is compared with that of diamond, AlN, quartz, and SiC (shown in Fig. 3). At $f > 3$ GHz, $f \cdot Q$ of $\langle 100 \rangle$ Si becomes comparable to that of SiC, which makes the realization of ultra-high-frequency high- Q resonators in silicon possible.

The equation for ω_τ (8) also suggests that high thermal conductivity materials such as diamond experience the Landau-Rumer effect at low frequencies. The measured data for $\alpha(\omega)$ of diamond [16] as well as the analytical calculation of ω_τ presented in [17] support this statement (see Fig. 3). Table 2 provides material constants for commonly used acoustic materials.

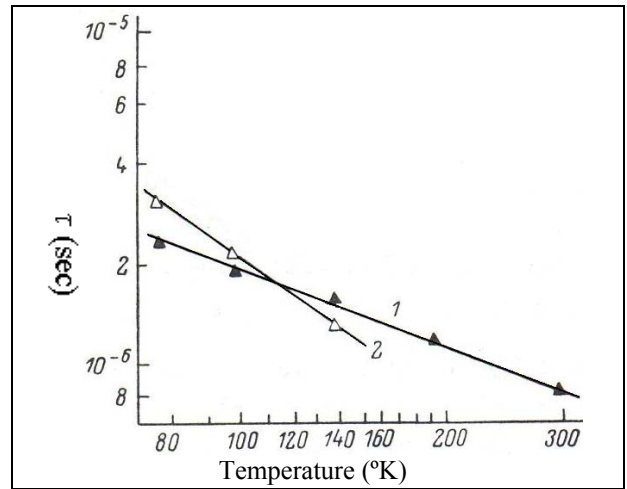


Figure 2. Temperature dependence of the acoustic phonon relaxation time (1) longitudinal in $\langle 100 \rangle$ and (2) longitudinal in $\langle 110 \rangle$ (figure reproduced from Reference [12]).

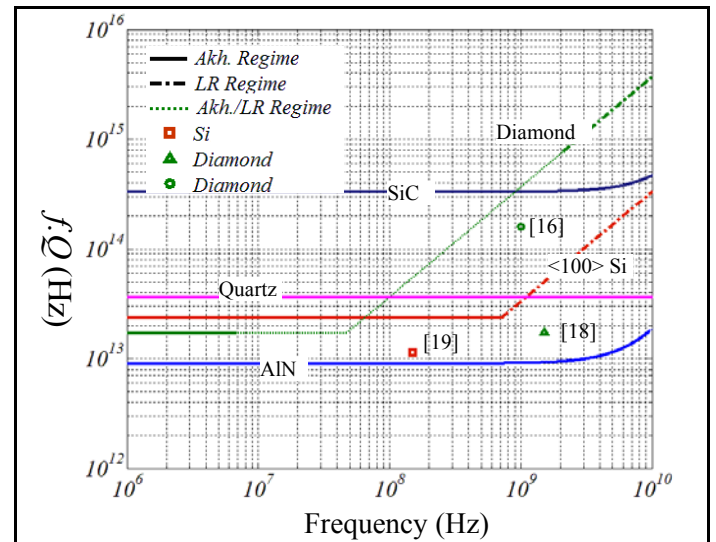


Figure 3. Comparison of $f \cdot Q_{PhP}$ of $\langle 100 \rangle$ Si with SiC, AlN, Quartz, and diamond. The highest $f \cdot Q$ product reported for Si and diamond resonators is presented in [18] and [19]. Reference [16] is from measured data for $\alpha(\omega)$ at 1 GHz.

Table 2. Intrinsic properties of some materials commonly used as micromechanical resonators. $\alpha(\omega)$ is the measured value for longitudinal. V_l is the velocity of the longitudinal wave.

	V_l (ms ⁻¹)	$\alpha(\omega)$ @ 1GHz (m ⁻¹)	β (μK ⁻¹)	κ (Wm ⁻¹ k ⁻¹)	C_v (Jcm ⁻³ k ⁻¹)
6H-SiC	13300	4.6	2.77	360	2.215
Si(100)	8500	69	2.57	130	1.631
Si(111)	9300	85	2.57	130	1.631
Si(110)	9100	83	2.57	130	1.613
Diamond	18000	6.9	1.05	2000	1.782
Quartz (C-axis)	5720	34.48	7.64	9.5	1.881
AlN	10970	200	2.56	162	1.938

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