Invited Article

Modification of Akhieser mechanism in Si nanomembranes and thermal conductivity dependence of the $Q$-factor of high frequency nanoresonators

E Chávez-Ángel$^{1,2}$, R A Zarate$^3$, J Gomis-Bresco$^1$, F Alzina$^1$ and C M Sotomayor Torres$^{1,4}$

$^1$Catalan Institute of Nanoscience and Nanotechnology (ICN2), Campus UAB 08193 Bellaterra (Barcelona), Spain
$^2$Dept. of Physics, Universitat Autònoma de Barcelona, Campus UAB, 08193 Bellaterra (Barcelona), Spain
$^3$Dpto de Física, Universidad Católica del Norte, UCN, Av. Angamos 0610, Antofagasta, Chile
$^4$Catalan Institution for Research and Advanced Studies (ICREA) 08010 Barcelona, Spain

E-mail: emigdio.chavez@icn.cat

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Abstract
We present and validate a reformulated Akhieser model that takes into account the reduction of thermal conductivity due to the impact of boundary scattering on the thermal phonons’ lifetime. We consider silicon nanomembranes with mechanical mode frequencies in the GHz range as textbook examples of nanoresonators. The model successfully accounts for the measured shortening of the mechanical mode lifetime. Moreover, the thermal conductivity is extracted from the measured lifetime of the mechanical modes in the high-frequency regime, thereby demonstrating that the $Q$-factor can be used as an indication of the thermal conductivity and/or diffusivity of a mechanical resonator.

Keywords: Akhieser nanoscale, thermal conductivity in membranes, $Q$-factor

(Some figures may appear in colour only in the online journal)

1. Introduction

Advances in nanofabrication methods have enabled the evolution from micro- to nano-electromechanical systems (MEMS and NEMS) with a vast variety of applications ranging from semiconductor technology to fundamental science [1]. MEMS- and NEMS-based oscillators have been used as extremely sensitive mass [2], force [3], charge [4] and spin [5] sensors. The coupling of MEMS and NEMS to the electromagnetic field via optical cavities, known as optomechanic cavities [6], has led to structures which provide quantum-limited displacement sensitivity [7] and back-action between photons and phonons. These characteristics of opto-mechanical structures have enabled the amplification of localized mechanical vibrations and the ensuing demonstration of phonon lasing [8], as well as ground state cooling at the nanoscale [9].

As the operation frequency of mechanical resonators enters the GHz regime [10–16], the intrinsic damping mechanism that arises from phonon-phonon scattering becomes dominant. It is precisely this mechanism that introduces a fundamental limit to the performance of the resonators, usually expressed by the ‘$Q \cdot f$’ product of the quality factor, $Q$, and the work frequency, $f$. Two different approaches, commonly referred to as Akhieser [17] and Landau–Rumer [18] models, have been used to describe the phonon-
phonon interaction damping processes. In the Akhieser model, the mechanical wave is treated as a macroscopic strain field in the crystal, which produces a shift of the equilibrium distribution of thermal phonons. The displaced thermal phonon distribution returns to equilibrium via phonon-phonon scattering, resulting in the time-dependent entropy of the system that leads to the absorption of the mechanical wave. In contrast, in the Landau–Rumer approach, all of the phonons are described as colliding individual particles, and the three-phonon scattering process is described by the Fermi golden rule, based on the quantum mechanical perturbation theory and the anharmonicity of the crystal potential. Therefore, it is important to consider the changes that arise from the reduction in feature size since phonon-phonon scattering depends on the materials’ properties. In the nanoscale, the shortening of the phonon mean free path (phonon lifetime) due to the diffusive scattering of phonons at the boundaries [19–22] reduces the thermal conductivity compared to the bulk value; as a consequence, the intrinsic damping mechanism (phonon-phonon scattering) is modified.

Although theoretical models are well established, a comparison with the experimental data is hindered by the number and uncertainty of the parameters used, including the thermal phonon mean free path and the Grüneisen parameter [23]. Moreover, accurate lifetime measurements of high-frequency phonons are a formidable task, and values remain unknown for most materials, with only a few reports on GHz for Si and GaAs [24–28].

Here, we report on the impact of size-dependent thermal properties on the intrinsic damping mechanism in a mechanical resonator; we take a free-standing silicon nanomembrane [29] as the simplest example of a nanoscale mechanical resonator. Such a membrane exhibits well-defined Lamb mechanical resonances with a thickness-tuneable frequency in the 10 GHz to 1 THz range. The intrinsic mechanical mode absorption is calculated using the Akhieser damping model [17], modified to take into account the size effect on the thermal conductivity due to thermal phonons that scatter at the boundaries. All of the simulations are compared against the experimental measurements in [25, 30].

Furthermore, we show that it is possible to extract the thermal conductivity from lifetime measurements, thus introducing the prospect of using measurements of the $Q$-factor to estimate the thermal conductivity and/or diffusivity of the resonator.

2. Modelling of the mechanical mode decay

The losses of the mechanical mode are divided into intrinsic and extrinsic contributions. While the first is related to the anharmonic decay, i.e. phonon-phonon scattering processes, the latter is due to scattering from defects, rough surfaces, interfaces, etc. The relative importance of these contributions varies with the temperature and the frequency of the mechanical mode.

For the intrinsic damping mechanism, we can distinguish two regimes of attenuation, namely Akhieser [17] and Landau–Rumer [18], which depend on the relationship between the phonon wavelength $\lambda$ and the averaged mean free path of thermal phonons, $\Lambda_{\text{mfp}}$. Although the frequencies of the thermal phonons span several decades, and their mean free path can vary over orders of magnitude [31, 32], a single parameter $\Lambda_{\text{mfp}}$ is usually defined to encompass the whole spectrum of the thermal phonons. Given this $\Lambda_{\text{mfp}}$, we can define an average thermal phonon lifetime as $\tau_{TH}=\Lambda_{\text{mfp}}/\bar{v}$, where $\bar{v}=(1/\nu_{f}^{3}+2/\nu_{s}^{3}+3)/3^{3/3}$ is the average Debye velocity, and $\nu_{f}$ is the longitudinal (transverse) velocity. $\tau_{TH}$ is linked to the thermal conductivity $\kappa$ through the expression in [33]

$$\tau_{TH} \approx \frac{3\kappa}{C_{V} \bar{v}^{2}}$$

where $C_{V}$ is the volumetric heat capacity. If the wavelength $\lambda$ of the acoustic wave is much larger than the typical averaged mean free path $\Lambda_{mfp}$ of the thermal phonons, i.e. $f \cdot \tau_{TH} \ll 1$, where $f$ is the frequency of the acoustic wave, we can assume that the acoustic wave interacts with the whole spectrum of the thermal phonons. This range is known as the Akhieser regime. On the other hand, if $\lambda$ is much less than $\Lambda_{mfp}$, i.e. $f \cdot \tau_{TH} \gg 1$, we describe the phonon attenuation using the Landau–Rumer formalism, and the phonon relaxation is assumed to be a three-phonon scattering process.

In the Akhieser regime, the intrinsic phonon relaxation rate of mode $s$ with angular frequency $\omega_s=2\pi f_s$ can be expressed as [17, 24, 34]

$$\tau_{\text{Ak}}^{-1}(\omega_s) = \frac{C_{V} T}{\rho v_s^2} \left( \frac{\omega_s^2 \tau_{TH}}{1 + \omega_s^2 \tau_{TH}^2} \right) \bar{v}^2$$

where $T$ is the temperature, $\rho$ is the mass density, $v_s$ is the group velocity of mode $s$ and $\bar{v}^2$ is the expected value of the square of the Grüneisen parameter taken over the entire spectrum of the thermal phonons. Due to the lack of direct experimental determination of $\gamma$ and $\tau_{TH}$, the alignment of the damping models has relied on the adjustment of these parameters to fit the experimental data [23]. In fact, the only direct measurement available of $\gamma$ is for modes that are a few high-symmetry points of the Brillouin zone [35]. The alternative is to infer $\gamma$ from density functional theory (DFT) calculations or by using the second- and third-order elastic constants [36]. In the case of $\tau_{TH}$, a kink in the slope of the mechanical mode attenuation-frequency plot is considered indicative of the frequency cut-off between the intrinsic damping regimes from which $\tau_{TH}$ is extracted [28, 38, 39]. However, it has been shown that this slope depends on the direction of the phonon propagation [23]. In [25], we showed that the Akhieser model did not describe the experimental data of the mechanical mode decay in the Si ultrathin membranes when a single value of $\tau_{TH}$ was used, regardless of the membranes thickness. As the real value of $\tau_{TH}$ is unclear, we used the constant value of $\tau_{TH}=17$ ps, taken from [24], which provided the best fit to the acoustic attenuation in the bulk silicon.

The thermal conductivity of the thin layers and membranes, $\kappa_{\text{film}}$, decreases appreciably compared to the bulk counterpart, $\kappa_{\text{bulk}}$. This reduction is mainly associated with the shortening of the phonon mean free path ($\Lambda_{\text{mfp}}$) and...
concomitantly with the phonon lifetime ($\tau_{TH}$) due to diffuse phonon scattering at the boundaries [19–22]. Introducing equation (1) in equation (2), the intrinsic phonon relaxation rate in the Akhieser regime can be rewritten as a function of the film thermal conductivity $\kappa_{film}$

$$\tau_{AK}^{-1} = 3T \frac{C_V}{\rho} \left( \frac{\bar{\gamma}}{\nu_s} \right)^2 \frac{a_0^2 (\kappa_{film}/C_V)}{(\bar{\gamma}^2 + (3a_0 \kappa_{film}/C_V)^2)^2} \gamma^2$$

(3)

or as a function of the thermal diffusivity $\alpha = \kappa_{film}/C_V$

$$\tau_{AK}^{-1} = 3TC_P \left( \frac{\bar{\gamma}}{\nu_s} \right)^2 \frac{a_0^2 \gamma^2}{(\bar{\gamma}^2 + (3a_0)^2)^2} \gamma^2$$

(4)

where $C_P$ is the specific heat capacity.

Following the approach by Ziman [39], the extrinsic processes are modelled using only the surface roughness scattering, $\tau_B$. The relaxation rate takes the form

$$\tau_B^{-1} (\omega_s) = \frac{\nu_s}{d} \frac{1 - p(\omega_s)}{1 + p(\omega_s)}$$

(5)

where $d$ is the thickness of the membrane, $\nu_s$ is the phonon group velocity of the mode and $p(\omega_s) = \exp(-4(\eta d / \nu_s)^2)$ is the fraction of phonons with frequency $\omega_s$ that undergo specular reflection at the boundaries characterised by roughness $\eta$.

The total lifetime $\tau_T$ of the specific mechanical mode of frequency $\omega_s$ can be obtained by combining the intrinsic and extrinsic contributions using Matthiessen’s rule

$$\tau_T^{-1} (\omega_s) = \tau_{intrinsic}^{-1} (\omega_s) + \tau_{extrinsic}^{-1} (\omega_s)$$

(6)

3. Results

Figure 1(a) shows the experimentally determined room-temperature thermal conductivity of Si membranes of thicknesses from ~400 nm to 9 nm [40–42], which undergo an appreciable decrease with decreasing the membrane thickness. The thermal conductivity model using the Fuchs–Sondheimer approach [43, 44] is seen to be in good agreement with the measured values. The details and parameters used in the simulation can be found in the supplementary information of [41].

An improved estimate of $\tau_{TH}$ can be obtained considering the thickness dependence of the thermal conductivity, $\kappa_{film}$, in equation (1). Figure 1(b) shows the calculated $\tau_{TH}$ as a function of thickness together with the constant values $\tau_{TH} = 17$ ps and 6 ps. While we took the first value ($\tau_{TH} = 17$ ps) from [24], where it was obtained as an adjustable parameter, the second value (6 ps) is directly derived from equation (2) by taking $\kappa_{film} = \kappa_{bulk} = 149$ W K$^{-1}$ m$^{-1}$ [45]. Then, once the dependence of $\tau_{TH}$ on the membrane thickness has been determined, we introduce the total effect on the intrinsic phonon attenuation through equation (3).

Finally, we calculate the total lifetime $\tau_T$ of the silicon membranes with consideration to the extrinsic surface-roughness boundary scattering $\tau_B$ and the intrinsic Akhieser damping effect $\tau_{AK}$. The values of $C_V$, $\bar{\gamma}$ and $\rho$ used in these simulations were taken from the literature [35]. Since the Grüneisen parameter in silicon fluctuates between $\pm 1$, depending on the direction and magnitude of the wavevector, it is possible to assume that the expected value of $\bar{\gamma}^2 = \langle \bar{\gamma}^2 \rangle = \langle \bar{\gamma}^2 \rangle^2$ is simply equal to 1. Although this approximation fails at low temperatures in which low-frequency phonons with similar values of $\bar{\gamma}$ are excited, at room temperature, most acoustic phonons are excited; therefore, the approach becomes reasonable [24]. Here, we consider only the first dilatational mode of the membrane; in this case, we can use the relation $\omega_s = \pi \nu_s / d$ to determine $\nu_s$. The value of $\eta = 0.5$ nm was taken from [25].

In figure 2, we compare the total relaxation time computed using the $\tau_{AK}$ discussed before and the three different values of the lifetime of the thermal phonons: two constant values ($\tau_{TH} = 17$ and 6 ps) and one thickness-dependent, given by equation (1). A better agreement with the experimental data is obtained with the last thickness-dependent. As pointed
In our previous work [25], we simulated the intrinsic damping in Si nanomembranes. This is exemplified in Si nanomembranes with mechanical mode frequencies above 10 GHz in which a Q-factor, depending on the mechanical mode and the thermal phonons, reaches its maximum. In other words, lowering the thermal conductivity results in the shift of the optimal mode attenuation to higher frequencies and, consequently, in an increase of the Q-factor for a range of frequencies up to \( f = 1/\tau_{TH} \). In other words, in low thermal conductivity resonators, the Q-factor at high frequencies will be limited intrinsically by the poor heat dissipation.

In the example considered here, which includes a Si membrane for which both the phonon lifetimes and thermal conductivities were already known, the validation of the modified Akhieser model becomes easier. Moreover, the connection established in the model between the mechanical mode lifetime and the thermal conductivity means that the thermal transport parameters could be obtained from the mechanical mode lifetime or from its Q-factor, but only if the pure Akhieser mechanism is the dominant damping loss. This is particularly advantageous for contactless optical methods, such as pump-and-probe [25, 26] or radio frequency spectroscopy [46] measurements, since standard electrical methods to measure \( \kappa \) require processing, and the calculations are not straightforward in complex shape nano/micro mechanical oscillators [47].

4. Conclusions

In this work, we have revisited the intrinsic damping mechanism that limits the performance of mechanical resonators in view of the modification of thermal properties in nanostructures. This is exemplified in Si nanomembranes with mechanical mode frequencies above 10 GHz in which a
reformulated Akhieser model is found to account very well for the measured decrease of the mechanical mode lifetime. We have demonstrated that for membranes, it is not possible to assume a constant thermal phonon lifetime irrespective of the membrane thickness since modifications of the thermal conductivity due to surface scattering must be taken into account. We show that the reduction of the thermal conductivity in nano-resonators, and consequently, a reduction of the thermal phonon lifetime, has a direct impact on the maximum $Q$-factor of a particular mechanical mode that, depending on the frequency range, could improve or degrade.

In addition, we suggest a method to extract thermal conductivity values from lifetime measurements, which opens the possibility to use the $Q$-factor as an indicator of the thermal conductivity and/or diffusivity of nano-resonators.

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