On the Air Damping of Micro-Resonators in the Free-Molecular Region

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ABSTRACT

Predicting air damping on micromachined mechanical resonators is crucial in the design of high-performance filters used in wireless communication systems. In the past, most of the work focuses on devices in which continuum theory can still be applied. In this work, we investigate damping on oscillating structures caused by air in the free-molecular region in which continuum theory is no longer valid. Such a study is important for devices operated at a very low pressure or for those whose characteristic length is on the order of nanometers. A careful examination of the previous work has been conducted. Mistakes and limitations have been found and reported in this paper. A molecular dynamics simulation has been developed and used in predicting quality factors of an oscillating micro beam operated at low pressures. Simulation results have shown an excellent agreement with experimental data.

Keywords: MEMS modeling, air damping, RF-MEMS

1 Introduction

There has been a lot of interest in using micromechanical resonator devices in wireless communication systems for various applications. One such example is to use them as high- frequency filters [1]. An electrostatically-driven, contour-mode disk resonator that oscillates at 733 MHz has been built [1]. Such designs have the potential to reach the gigahertz frequency range. A critical performance criterion of these resonators is the quality factor. A high quality factor is highly desirable in order to achieve high sensitivity. For this reason, there has been extensive research on investigating air damping on resonators [2,3]. Most of the studies focus on the devices with minimum feature size on the order of microns. At micro scale and standard pressure, continuum theory is still valid and was employed in the previous studies. In this work, we investigate air damping on resonators when the surrounding gas (air) is in the free-molecular region (Knudsen number > 10). This situation becomes important when resonators are operated at a very low pressure or the minimum feature size of the devices is on the order of nanometers. An application of this work could be the design of a gigahertz disk resonator for which the gap between the resonator and the surrounding electrodes has to be in the submicron range (80 nm - 1 nm) in order to drive the stiff disk into resonance. With such a small gap, continuum theory breaks down and a molecular approach that accounts for interactions between the disk and individual molecules must be adopted.

Previous work on using molecular approaches to study air damping has been focused on micro-beam resonators operated at a very low pressure [4,7,8,9]. During the course of this study, we have found errors and limitations of these approaches. A molecular dynamic simulation has been developed to find the quality factor of the micro-beam resonator. With this approach, a much improved agreement with the experimental measurements has been achieved.

This paper is organized as follows. In the next section, a brief introduction of previous studies of air damping on a micro-beam resonator is given. It is followed by a careful examination of the previous approaches and corrections. In Section 3, the molecular dynamics simulation is described and the simulation results are presented.

2 The Theoretical Analysis of Micro-Beam Resonators

Previous work involving the analytical derivation of the damping effect on an oscillating beam was done by Christian [4], Kadar et al. [7], Li et al. [8], and Bao et al. [9]. Christian proposed a free molecular theory that was used to calculate the damping force acting on an oscillating vane in a vacuum by finding the pressure difference between the front and back of the vane using the Maxwell-Boltzmann speed distribution function for gases [4]. When this model was used to compute the quality factor of a micro-beam resonator, the quality factor was almost one order higher than the experimental results [6]. In an attempt to bring the theoretical values closer to the measurements, Kadar introduced a modification to Christian's method that involved a new molecule speed distribution function (the Maxwellian-Stream distribution), reducing Christian's quality factor results by a factor of π [7]. Li modified Kadar's Maxwellian-Stream (MS) distribution function to ac-

count for the velocity of the contact surface [8]. This further reduced Kadar's quality factor results, bringing the analytical solution even closer to the experimental results of Zook [6]. By pointing out the importance of the effects of damping caused by a nearby wall and the redundancy in Kadar's velocity distribution function, Bao introduced the energy transfer model as a way of directly calculating the energy loss [9]. He has shown that his results are closer to the experimental results than those based on Christian's model.

2.1 Errors in Kadar's Modification

Despite good agreements with experimental measurements, there are two fundamental mistakes in Kadar's approaches. As pointed out by Bao [9] (although without explanation), the Maxwellian-Stream distribution function is used redundantly. The redundancy comes from the way the number of molecules striking the microbeam is computed. In Christian's model, it is calculated by constructing a control volume of $V = v_r dA dt$, where v_r is the relative velocity between the gas molecule (v) and the beam (u), dA and dt are the striking area and time respectively. Thus, the density of molecules that strike the beam within time dt and area dA is

$$n \cdot \int_0^\infty V \cdot MB(v) dv$$

where $MB(v) = \left(\frac{m}{2\pi kT}\right)^{\frac{1}{2}} \exp -\frac{mv^2}{2kT}$ is the Maxwell-Boltzmann (MB) distribution function, m is the mass of the gas molecule, k is Boltzmann's constant, T is the absolute temperature of the gas, and n is the density of molecules. In Kadar's model, the Maxwellian-Stream (MS) distribution is used instead. Unlike the MB function that gives the velocity distribution of all the molecules in a general gas assembly, the MS function is the velocity distribution function of the molecules that strike the surface. Thus, when using MS to calculate the density of molecules that strike the micro-beam, the correct value should be $n \cdot \int_0^\infty MS(v) dv$. However, in Kadar's calculation, it is $n \cdot \int_0^\infty V \cdot MS(v) dv$. Kadar simply replaced the MB distribution function with the MS distribution function in Christian's calculation, which is not correct.

A second mistake comes from the coefficient in the MS distribution function used in Kadar's model. Directly adopted from [10], the coefficient in $C(c)$ is $\frac{1}{2}\left(\frac{m}{kT}\right)^2$ ([7], equation (12)). This coefficient, however, is obtained by considering only the molecules that strike the surface, i.e., integrating this distribution function in the velocity space gives only the total number of molecules that strike the surface, not the total number of gas molecules as a whole. The correct coefficient should be $\frac{m}{2kT}\sqrt{\frac{m}{2\pi kT}}$. With this coefficient and the correct way of computing the density of molecules that strike the surface using the MS distribution function, the net pressure acting on the micro beam is

$$p = 2m \int_0^\infty [n \cdot \sqrt{\frac{m}{2\pi kT}} e^{-\frac{mv^2}{2kT}} (v+u)^2 - n \cdot \sqrt{\frac{m}{2\pi kT}} e^{-\frac{mv^2}{2kT}} (v-u)^2] dv. \quad (1)$$

After taking the common factors out of the integral, the above equation corresponds exactly with the pressure equation derived from Christian's model (shown in equation (12) in [4]). This is not surprising since the fundamental principle used in Christian's and Kadar/Li's approaches is exactly the same.

2.2 Limitations of Bao's Energy Transfer Model

In [9], Bao et al. used a direct approach to determine the energy transfer between a resonating device and the equilibrium gas that surrounds it. By assuming elastic collisions between gas molecules and a resonating structure and ignoring the intermolecular collisions, Bao's model uses energy transfer mechanics to calculate the kinetic energy gain of molecules and therefore obtain the quality factor of the resonator structure. By applying this model to the oscillating micro beam, Bao was able to show that the calculated quality factor compared favorably with the measurements from Zook's microbeam experiment. Because it incorporates nearby walls and device geometry, Bao's energy transfer model provides a reasonable starting point for the analysis of resonating MEMS devices with various geometries. However there are three prevailing assumptions in the development of Bao's model. The first is that the velocity change of each particle is only considered after collisions with the resonating device have occurred; that is, the velocity of each particle is assumed to be constant for the entire period of interaction with the disk. This allows for a much simpler expression for the number of collisions ΔN, given by (2)

$$\Delta N = \frac{\Delta t \times v_{xo}}{2(d_o - x)} = \frac{l v_{xo}}{2(d_o - x) v_{yzo}} = \frac{l}{2\sqrt{2}(d_o - x)} \quad (2)$$

where Δt is the time a gas molecule is within the region where it can interact with the device, l is the distance the molecule travels in the region, d_o is the initial gap between the device and the stationary wall, x is the displacement of the device as it oscillates, and v_{xo} and v_{yzo} are the initial velocities of the molecule in the x- and yz-directions, respectively. This implies that the number of collisions of a gas molecule whose velocity increases each time when it collides with the beam is the same as that of a molecule whose velocity decreases each time when it collides with the beam. Such an assumption could largely underestimate the energy gained by the gas molecules since the number of collisions of molecules

who gain velocity is larger than the number of collisions of molecules who loss velocity. Figure 1 illustrates this

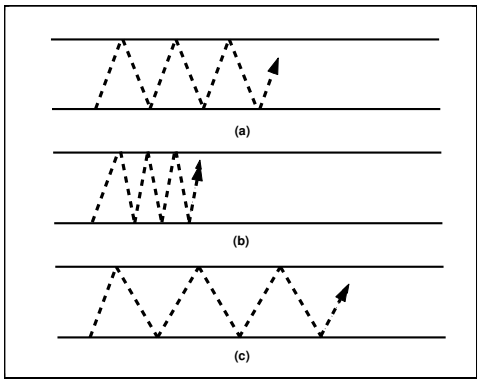

Figure 1: The Effects of the "Constant Velocity" Assumption

idea. In Figure 1(a), the path of a molecule is shown in time. This molecule's motion is based on the assumption that it continues with its initial velocity after every collision. Figures 1(b) and 1(c) show that if the velocity of the molecule increases or decreases after each collision, the time between two consecutive collisions will decrease or increase. For the same travel time (determined by l and v_{yzo}), the number of collisions will therefore be different. Since the final velocity of the molecule is based on the number of collisions ΔN, a change in this number will change the kinetic energy. As shown in the results section, this change is quite significant.

The second assumption is that the amplitude of the device's motion is much smaller than the gap between the moving device and any nearby walls. By this assumption, the device can be seen as stationary (distancewise), thus further simplifying the calculation for the number of collisions that each molecule will have with the device to a constant. This assumption follows logically from the geometry and actuation mechanisms of the devices being studied.

The third major assumption is that the time for a gas molecule staying under the micro-beam (travel time) is much smaller than the oscillating cycle of the beam. Therefore, the velocity gained or lost by a molecule after each collision remains the same during its travel time. This is valid for the micro-beam being studied, as the oscillating period of the beam is almost one order smaller than the travel time of a molecule under the beam.

3 Molecular Dynamics Simulation

3.1 The MD Simulation

In order to develop a general approach to calculate the energy transferred between a resonating device and the gas surrounding it, a one-dimensional molecular dynamics simulation has been developed. The simulation tracks the position and velocity of one molecule as it moves within the gap between the device and nearby walls for a fixed period of time. Collisions between the molecule and the device or walls are assumed to be elastic and the energy transferred during the collision is calculated based on energy transfer mechanics, which incorporate the conservation of momentum and conservation of kinetic energy laws. The change of velocity of the molecule during each collision is recorded and the final velocity is obtained by adding the cumulative changes of velocity to the initial value. The final kinetic energy of the molecule was then calculated. To compute the total energy gained by the molecules during one oscillating cycle of the beam, the cycle is divided into many intervals (Δt). The changes of energy for molecules entering into the gap within each time interval are calculated and results are added to obtain the total energy change as shown in equation (3),

$$\Delta E_{cycle} = \frac{1}{4} n \bar{v} L \left(\sum \Delta e_k \right) \Delta t \tag{3}$$

where $\bar{v}$ is the average velocity of the molecule, L is the peripheral length of the beam, and Δe_k is the change in kinetic energy of the molecule at each period division (Δt). The quality factor Q of the device was then calculated according to equation (4).

$$Q = \frac{2\pi E_B}{\Delta E_{cycle}} = \frac{2\pi \frac{1}{2} m_B A_0^2 \omega^2}{\Delta E_{cycle}} \tag{4}$$

where m_B is the mass of the beam, A_0 is the amplitude of the beam displacement, and ω is the natural frequency.

3.2 Results - Quality Factor

To verify our MD simulation, the energy loss of the beam during one cycle was simulated first following exactly the same assumptions employed in Bao's model. The quality factors were calculated at different discretizations of the period (i.e., the different division of the period) and shown in Figure 2. As can be seen by Figure 2, the simulation results for Q_{sim} converge very closely to the value calculated from Bao's model (Q_{Bao}). The lower curve in Figure 2 (Q_{simV}) shows the resulting values when the molecular velocity is updated after each collision, instead of after the end of the travel time. It can be seen that the value converges to a little less than half of Bao's theoretical value. It is from this drop in quality factor that we can say that the "constant velocity" assumption made by Bao is incorrect. Figure 3 shows these results as compared to Zook's experimental and Christian's and Bao's theoretical results. Although

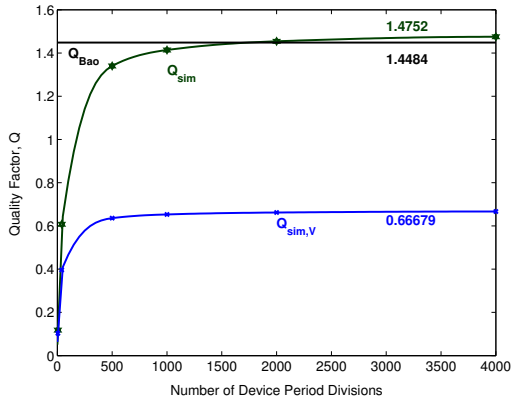

Figure 2: Convergence of Simulation Results

based on free-molecular assumption Bao's results most closely approximate the experimental values in the pressure range between 10^1 torr and 10^3 torr. At this range, the corresponding Knudsen number is between 4.4 and 0.044, indicating that the gas is in the transition or slip region in which the intermolecular collisions are important. The results from the simulation where the constant velocity assumption was relaxed show that the calculated values agree well with the experimental values in the pressure region lower than 10^1 torr (i.e., the Knudsen number is higher than 4.4) which is consistent with the assumption of free molecular region used in this study.

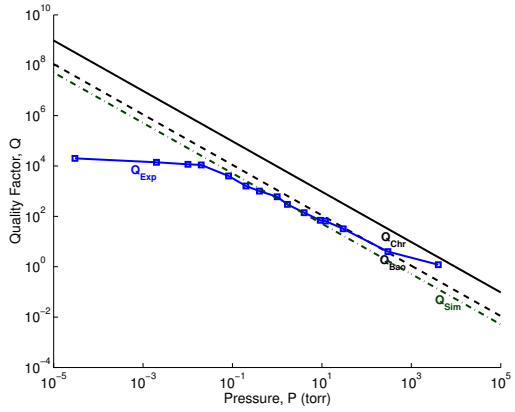

Figure 3: Simulation Results

4 Conclusion

In this paper, we report our studies on damping of oscillating microstructures caused by air in the free-molecular region. Previous work has been carefully examined and mistakes were found in Kadar/Li's approach. By correcting the mistakes, we demonstrate in this paper that Kadar/Li's approach leads to the same conclusion as that of Christian's which is valid for a structure oscillating in a free space. For structures oscillating near a fixed wall such as the micro beam being studied, Bao's model is much more appropriate than Christian's. However, we also found that the "constant velocity" assumption used in Bao's model led to a much smaller energy loss prediction in the oscillating micro beam. To relax this assumption and to develop a general approach, a molecular dynamic simulation has been developed and used to obtain the quality factors of a oscillating micro beam operated at very low pressures. Results have shown an excellent agreement with the experimental data, particularly in the free-molecular region.

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