A Macro Model of Squeeze-Film Air Damping in the Free-Molecule Regime

Gang Hong and Wenjing Ye

Citation: AIP Conference Proceedings **1233**, 219 (2010); doi: 10.1063/1.3452169
View online: http://dx.doi.org/10.1063/1.3452169
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1233?ver=pdfcov
Published by the AIP Publishing

A Macro Model of Squeeze-Film Air Damping in the Free-Molecule Regime

Gang Hong[a] and Wenjing Ye[a, b, *]

[a]*Department of Mechanical Engineering, Hong Kong University of Science and Technology*
[b]*KAUST-HKUST Micro/Nanofluidic Joint Laboratory*
(mewye@ust.hk)*

Abstract. An accurate macro model for free-molecule squeeze-film air damping on micro plate resonators is present. This model relates air damping directly with device dimensions and operation parameters and therefore provides an efficient tool for the design of high-performance micro resonators. The construction of the macro model is based on Molecular Dynamics (MD) simulations and analytical traveling-time distribution. Its accuracy is validated via the comparison between the calculated quality factors of several micro resonators and the available experimental measurements and full MD simulation results. It has been found that the relative errors of the quality factors of two resonators, as compared with experimental data, are 3.9% and 5.7% respectively. The agreements between the macro model results and MD simulation results, on the other hand, are excellent in all cases considered.

Keywords: Squeeze-film damping, free-molecule regime, resonator, quality factor.
PACS: 47.45.Dt, 85.85.+j, 47.11.Mn

INTRODUCTION

Energy dissipation is one of the most important factors that affect a micro resonator's performance. Among various damping mechanisms, air damping could be a significant source even when the device is packaged in a medium vacuum. This fact has led to a series of work on the development of models and numerical tools for the prediction of air damping of resonant structures [1-10]. While methods for the prediction of squeeze-film air damping in the continuum and near-continuum regimes are quite mature, the same can not be said to the models suitable for the free-molecule and transition regimes where the mean free path of gas molecules is comparable or larger than the characteristic length. A major hurdle is the breakdown of the continuum theories at these regimes which prohibits the use of many well-developed methods.

Significant efforts have been made towards the extension of continuum-based methods to account for rarefaction effects on the squeeze-film damping in these regimes [5,6,7]. Examples include, but are not limited to, the modification of the Reynolds equation by employing the effective viscosity [5], the pressure dependent effective flow rate coefficient [6] and a modified pressure boundary condition with coefficients extracted from the Navier-Stokes slip-jump simulations and the direct simulation Monte Carlo simulations [7]. Most of these methods have demonstrated their accuracy in the slip regime ($Kn \le 0.1$), i.e., the near continuum regime. Their applicability in the free-molecule regime, however, is yet to be demonstrated. Veijola, *et al*'s 1995 model [5] was claimed to be accurate for a wide range of Knudsen number ($0 \le Kn \le 880$), but it fails to capture the linear relationship between air damping and the ambient pressure in the free-molecule regime.

Models and approaches based on individual molecular transport have also been developed [8,9,10]. The analytical squeeze-film damping model proposed by Bao, *et al* [9] employs several assumptions. Unfortunately some of them are not accurate and can cause large errors in some cases [10]. A semi Molecular Dynamics (MD) approach which tracks the motion of a representative particle and its collisions with oscillating resonator was employed [10] to model air damping. Although the semi-MD approach has brought the prediction of air damping of Zook's resonator [11]

much closer to the experimental data than Bao's model , due to the use of one representative particle instead of many real particles in the simulation, the accuracy of this approach depends on the choice of the representative particle. A full MD simulation would improve the accuracy greatly. However, the major bottleneck of such a method is the required massive computational power, which prohibits its use in a practical design tool.

This paper presents a macro model of squeeze-film air damping on a rectangular plate/beam resonator in the free-molecule regime. The objective of this work is to develop an accurate model which correlates damping directly with device dimensions and operation parameters to provide an efficient design tool. The macro model was developed based on the analytical density function of molecular interaction time and MD simulations. The basic assumptions employed in the model are (1) elastic collisions between gas molecules and resonators and (2) rigid motion of resonators.

AIR DAMPING MODEL

The energy loss of the resonator is determined by the collisions between gas molecules and the resonator, which in turn depends on the time each molecule stays within the interaction region, and energy exchange between molecules and resonator at each collision. Consider a cycle at which the system (resonator and gas) has reached its quasi-steady state and denote it as the *N*th cycle. The energy loss of the resonator within this cycle, $\Delta E^{(N)}$ can be written as $\Delta E^{(N)} = \sum_{j=1}^{j=N} \Delta E_1^{(j)}$, where $\Delta E_1^{(j)}$ is the energy damping due to the collisions between the resonator and gas molecules that enter the interaction domain within the *j*th cycle. Without losing generality, assume the resonator is at its equilibrium position at the beginning of the *N*th cycle. The position of the resonator during one period is $x = d - A\sin\omega u$, where d is the initial gap between the resonator and the nearby fixed wall, A and ω are the oscillation amplitude and angular frequency respectively . The number rate of molecules entering the interaction domain at time u is $\frac{1}{4} n\bar{V}Lx$, where n is the number density, $\bar{V} = \sqrt{\frac{8kT}{\pi m}}$ is the average speed of gas molecules in the surrounding reservoir, m is the molecular mass, k is the Boltzmann constant, T is the temperature and L is the peripheral length of the resonator. Among them, the number rate of molecules whose traveling time falls within the range of $(t,\ t+dt)$ is $\frac{1}{4} n\bar{V}L\left(d - A\sin\omega u\right) f(t)\,dt$, where $f(t)$ is the normalized probability density function of molecular traveling time, t. Let $e_{u,t}$ be the average energy change of these molecules. The expression of $\Delta E^{(N)}$ can be obtained by summing up the contributions of all molecules with their traveling times in the range of $(0,\ \infty)$. It reads

$$\Delta E^{(N)} = \frac{1}{4} n\bar{V}L dT_o \frac{kT}{4\pi} \int_0^\infty \Delta\bar{E}_t f(t)\,\mathrm{d}t \ , \tag{1}$$

where $\Delta\bar{E}_t = \frac{2\pi}{kT/2} \int_0^{T_o} \frac{1}{T_o} \left(1 - \frac{A}{d}\sin\omega u\right) e_{u,t}\,\mathrm{d}u$ represent the normalized average energy change of molecules with traveling time of t.

Normalized Average Energy Change of Molecules With Traveling Time Of t: $\Delta\bar{E}_t$

In order to develop an accurate analytical expression for $\Delta\bar{E}_t$, a three-dimensional molecular dynamics simulation code has been developed. The simulation tracks the motion of each gas molecule during its interaction with the moving structure and uses the conservation of linear momentum and conservation of kinetic energy to calculate the change of velocity and thus the energy gain or loss of the molecule after each collision. In an elastic-collision event, the tangential velocity of a gas molecule remains unchanged. The normal velocity gains a velocity of $2|V|$ in a head-on collision, while in a head-tail collision event, it losses or gains a velocity of $2|V|$ depending on the relative speed of gas molecule and resonator. Figure 1 illustrates the computational domain of the MD simulation. The top plate represents the oscillating resonator and the bottom plate represents the fixed wall. The cuboid confined between the two plates is the interaction region. Gas molecules enter the interaction region from the surrounding stationary gas reservoir, which is assumed to be at equilibrium. After interacting with plates, they leave the interaction region without being re-introduced on the opposite side. This allows the finite-size effect of the device to be modeled. To

improve efficiency, a surface generation algorithm was employed [12]. Molecules are emitted into the interaction region from its open boundary at a rate that is determined by gas density and temperature at the surrounding reservoir. Their initial positions are uniformly distributed along the boundary. The normal velocity of these molecules follows the one-sided Maxwell-Boltzmann velocity distribution and their parallel components follow the ordinary Maxwell-Boltzmann distribution.

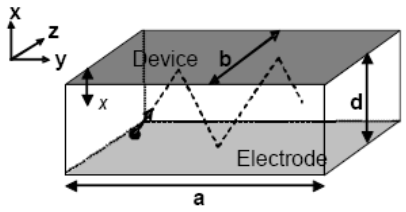

FIGURE 1. MD simulation domain.

MD simulations are conducted to identify the key non-dimensional parameters that influence air damping. It has been found that among all the parameters, $\Delta\bar{E}_t$ is fully characterized by two non-dimensional parameters, $r = A/d$ and $\tau = \omega t$. The relationships between air damping and the two non-dimensional parameters obtained from MD simulations suggest that a suitable function form of $\Delta\bar{E}_t$, which is a function of *r* and τ, is

$$\Delta\bar{E}_t = \Delta\bar{E}(r,\tau) = r^2 \sin^2\frac{\tau}{2}\cdot y(r,\tau);\ y(r,\tau) = P_0 + \alpha(r)\sin^2\frac{\tau}{2} + \beta(r)\left[\tau - (2k+1)\pi\right]^2;\ 2k\pi \le \tau \le 2(k+1)\pi .$$

The parameters P_o, $\alpha(r)$, $\beta(r)$ are determined based on the values of *y* at $\tau = (2k+1)\pi$ and $\tau = 2k\pi$, as shown in Figure 2.

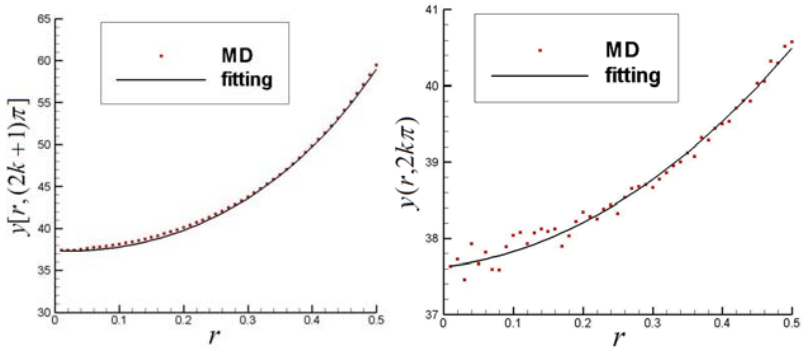

FIGURE 2. Dependence of $y(r,\tau)$ on r at $\tau = (2k+1)\pi$ (left) and $\tau = 2k\pi$ (right).

The least-square fitting of these data yields

$$P_0 = 37.37,$$
$$\alpha(r) = P_0\left[\exp(2.115r^2 - 0.089r) - 1\right],$$
$$\beta(r) = P_0\left[\exp(0.235r^2 + 0.031r + 0.0068) - 1\right]/\pi^2 .$$

The average energy change of molecules with a traveling time of τ is thus

$$\Delta\bar{E}(r,\tau) = r^2\sin^2\frac{\tau}{2}\left\{P_0 + \alpha(r)\sin^2\frac{\tau}{2} + \beta(r)\left[\tau - (2k+1)\pi\right]^2\right\}. \qquad (2)$$

Probability Density Function of Molecular Traveling Time

Due to elastic collisions, the in-plane velocities of a gas molecule remain constant during its interaction with the resonator. Hence, the traveling time of each molecule depends solely on its in-plane velocity, initial location and plate geometry. The probability density function of the traveling time is obtained by first finding the density function

of the traveling distance determined by the location at which the gas molecule enters the interaction region and the in-plane traveling direction. The distribution of gas molecules' initial locations is uniform along the boundary of the interaction region. In addition, the velocity distributions of these molecules imply that the probability density function of the traveling direction, represented by the polar angle θ as shown in Figure 3, is $\sin\theta$.

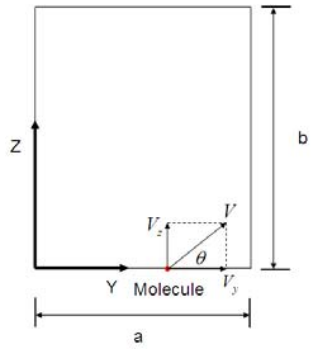

FIGURE 3. The top view of a plate resonator with a gas molecule locating at the entrance.

Based on these distributions, the probability density function of the traveling distance is obtained as

$$f_{L^*}(l)=\begin{cases}\dfrac{1}{1+\gamma} & 0<l\le 1\\ \dfrac{1}{1+\gamma}\dfrac{\gamma}{l^2\sqrt{l^2-1}} & 1<l\le\gamma\\ \dfrac{1}{1+\gamma}\left[\dfrac{1}{l^2}\left(\dfrac{\gamma^2}{\sqrt{l^2-\gamma^2}}+\dfrac{\gamma}{\sqrt{l^2-1}}\right)-1\right] & \gamma<l\le\sqrt{1+\gamma^2}\end{cases}, \quad (3)$$

where $\gamma=b/a$ is the aspect ratio of the plate dimensions and *l* denotes the traveling distance.

Traveling time of a gas molecule is the ratio of its traveling distance and its in-plane speed. The in-plane molecular speed has a probability density function of $f_{V_{yz}}(v_{yz})=\sqrt{\frac{2}{\pi}}(\frac{m}{kT})^{3/2}v_{yz}{}^2\cdot e^{-\frac{mv_{yz}{}^2}{2kT}}$, $0\le v_{yz}<+\infty$. In the non-dimensional form, this density function is $f_{V^*}(v)=c\cdot f_{V_{yz}}(cv)=\sqrt{\frac{2}{\pi}}v^2\cdot e^{-\frac{v^2}{2}}$, $0\le v<+\infty$, where $V^*=V_{yz}/c$ is the non-dimensional in-plane speed and $c=\sqrt{kT/m}$. With the probability density functions of both traveling distance and speed, the distribution function of the non-dimensional traveling time, defined as $T_t^*=L^*/V^*$, can be deduced as

$$f_{T^*}(t)=\frac{1}{1+\gamma}\left[-\frac{e^{-\frac{1}{2t^2}}}{t^3}\left[\sqrt{\frac{2}{\pi}}t(1-e^{-\frac{\gamma^2}{2t^2}})-\gamma\,\mathrm{Erf}(\frac{\gamma}{2t})\right]+2\sqrt{\frac{2}{\pi}}(1-e^{-\frac{\gamma^2}{2t^2}})(1-e^{-\frac{1}{2t^2}})-\frac{\gamma^2e^{-\frac{\gamma^2}{2t^2}}}{t^3}\left[\sqrt{\frac{2}{\pi}}t(1-e^{-\frac{1}{2t^2}})-\mathrm{Erf}(\frac{1}{2t})\right]\right] \quad 0\le t<+\infty \quad (4)$$

RESULTS

Validation of the MD Code

A recent experiment conducted by Sumali [13] was chosen to validate the developed MD simulation code. In Sumali's experiment, an electro-deposited gold micro-plate resonator was fabricated which oscillates perpendicularly to the substrate at a frequency of 16.91 kHz and at an amplitude of 0.1 μm. The main structure component of the resonator is a central plate suspended above the substrate by four folded beams as shown in Figure 4. The geometry of central plate is approximated as a rectangle plate with dimensions of $a=154.3\mu m$ and $b=196.2\mu m$, which were

chosen to match its area. The thickness of the plate is 5.7 μm and the initial gap between the plate and the substrate is 4.1 μm.

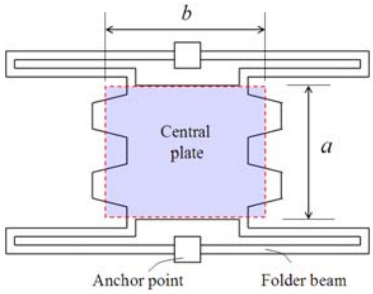

FIGURE 4. (a) Solid model of a pressurized thick cylinder, (b) BEM mesh with 950 panels.

Energy changes of gas molecules within one cycle were computed using the MD code at various ambient pressures. The quality factors of the device, defined as $Q = \frac{\pi M (A\omega)^2}{\Delta E}$, where M is the mass of the resonator, were computed and plotted in Figure 5 together with Sumali's experimental measurements. Also shown in the figure are the results obtained from Bao's model and semi-MD simulation. Clearly MD simulation gives the most accurate prediction of the quality factor in the free-molecule regime which corresponds to a pressure range of 130 Pa and lower.

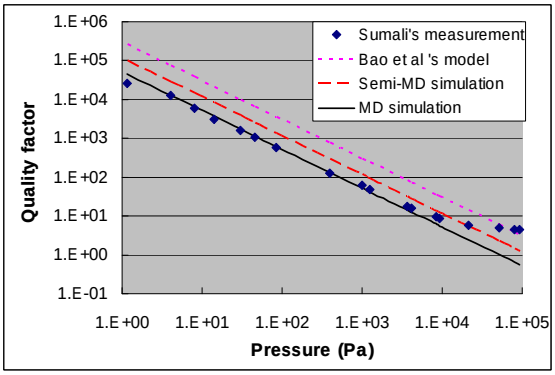

FIGURE 5. Comparison of different modeling approaches and Sumali's measurement.

Validation of the Macro Model

With the analytical expressions for $f(t)$ (Equation 4) and $\Delta\bar{E}(\tau, r)$ (Equation 2), the energy damping of a plate resonator can be evaluated via numerical integration of Equation (1). Due to the rapidly decayed density function $f(t)$, a finite integration range, typically from zero to a few periods, is sufficient to yield accurate results. In the following examples, the maximum upper limit used in the calculation is two oscillation periods. The error introduced by replacing the infinite upper limit with $2T_o$ is less than 0.1%.

Table 1 lists the parameters of several testing resonators. The first two are real devices [11,13], for which the measured quality factors are available. The rest three were arbitrarily constructed to test various combinations of parameters. The products of the quality factor and ambient pressure obtained from the derived macro model and MD simulations are listed in Table 2. Also shown are the experimental data for the first two resonators. The agreement between the MD results and the macro-model results is excellent. In all cases the relative errors between the two sets of results are less than 1%, indicating that the simple macro model has faithfully reproduced the MD results for a wide range of plate resonators. The relative errors between the measured data and macro-model results are 3.9% and 5.7% respectively, much smaller than the errors produced by any other existing models.

TABLE 1. Parameters of various testing resonators

	a	*b*	*d*	*A*	*f*	*T*
Unit	μm	μm	μm	μm	KHz	K
Zook *et al*'s resonator	40	200	1.1	0.11	550	273
Sumali's resonator	154.3	192.6	4.1	0.1	16.91	295
Resonator No. 3	2	500	1.2	0.12	500	273
Resonator No. 4	50	250	2.5	0.5	100	273
Resonator No. 5	100	100	6	0.3	50	273

TABLE 2. Q*P of various resonators

	Macro Model	MD Simulation	Measurement
Zook *et al*'s resonator	401	399	386
Sumali's resonator	384	387	366
Resonator No. 3	76242	75510	
Resonator No. 4	2356	2352	
Resonator No. 5	2575	2554	

SUMMARY

A macro model for squeeze-film air damping in the free-molecule gas regime has been developed for rectangular plate resonators. This model relates air damping directly with device parameters and hence provides an efficient tool for the design of micro resonators with high quality factors. The accuracy of the model was validated by both MD simulations and experimental measurements. Very good agreements have been obtained for a wide range of resonators.

ACKNOWLEDGMENTS

The contents presented in this paper were supported in part by Hong Kong Research Grants Council under Competitive Earmarked Research Grant 622109 and in part by Award No. SA-C0040/UK-C0016, made by King Abdullah University of Science and Technology. Their financial support is gratefully acknowledged.

REFERENCES

1. M. Andrews, I. Harris and G. Turner, "A comparison of squeeze-film theory with measurements on a microstructure," Sens Actuators A Phys, 36, pp 79-87, (1993).
2. Y. J. Yang and S. D. Senturia, "Numerical simulation of compressible squeezed-film damping," in Proceeding of Solid-State Sensor and Actuator Workshop, pp 76-79, (1996).
3. G. Schrag and G. Wachutka, "Physically based modeling of squeeze film damping by mixed-level system simulation," Sens Actuators A Phys, 97-98, pp 193-200, (2002).
4. M. Bao, H. Yang, Y. Sun and P. J. French, "Modified Reynolds' equation and analytical analysis of squeeze-film air damping of perforated structures," J Micromech Microengineering, 13, pp 795-800, (2003).
5. T. Veijola, H. Kuisma, J. Lahdenpera and T. Ryhanen, "Equivalent-circuit model of the squeezed gas film in a silicon accelerometer," Sens Actuators A Phys, 48, pp. 239-248, (1995).
6. T. Veijola, "Compact models for squeezed-film dampers with inertial and rarefied gas effects," J Micromech Microengineering, 14, pp. 1109-1118, (2004).
7. M. A. Gallis and J. R. Torczynski, "An improved Reynolds-equation model for gas damping of microbeam motion," *J Microelectromech Syst*, vol. 13, pp. 653-659, (2004).
8. R. Christian, "The theory of oscillating-vane vacuum gauges," Vacuum, 16, pp. 175-178, (1966).
9. M. Bao, H. Yang, H. Yin and Y. Sun, "Energy transfer model for squeeze-film air damping in low vacuum," J Micromech Microengineering, 12, pp. 341-346, (2002).
10. S. Hutcherson and W. Ye, "On the squeeze-film damping of micro-resonators in the free-molecule regime," J Micromech Microengineering, 14, pp. 1726-1733, (2004).
11. J. D. Zook, D. W. Burns, H. Guckel, J. J. Sniegowski, R. L. Engelstad and Z. Feng, "Characteristics of polysilicon resonant microbeams," Sens Actuators A Phys, 35, pp. 51-59, (1992).
12. M. W. Tysanner and A. L. Garcia, "Non-equilibrium behaviour of equilibrium reservoirs in molecular simulations," Int. J. Numer. Methods Fluids, 48, pp. 1337-1349, (2005).
13. H. Sumali, "Squeeze-film damping in the free molecular regime: Model validation and measurement on a MEMS," J Micromech Microengineering, 17, pp. 2231-2240, (2007).