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Citation: [Physics of Fluids \(1994-present\)](#) **22**, 012001 (2010); doi: 10.1063/1.3275844

View online: <http://dx.doi.org/10.1063/1.3275844>

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A macromodel for squeeze-film air damping in the free-molecule regime

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(Received 24 June 2009; accepted 20 October 2009; published online 7 January 2010)

A three-dimensional Monte Carlo (MC) simulation approach is developed for the accurate prediction of the squeeze-film air damping on microresonators in the free-molecule gas regime. Based on the MC simulations and the analytical traveling-time distribution, a macromodel, which relates air damping directly with device dimensions and operation parameters, is constructed. This model provides an efficient tool for the design of high-performance microresonators. The accuracy of the macromodel is validated through the modeling of the quality factors of several microresonators. 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 macromodel results and MC simulation results, on the other hand, are excellent in all cases considered. © 2010 American Institute of Physics. [doi:10.1063/1.3275844]

I. INTRODUCTION

Modeling of squeeze-film air damping encountered in microelectromechanical systems devices has been an active research topic due to (1) its importance in the prediction of the quality factors of microresonators, an important measure of the performance of these devices, and (2) the challenges in the modeling of rarefied gas transport.^{1–25} When resonators operate in air, their quality factors are often determined by the level of air damping, a dominant dissipation source for most devices. Methods for the reduction in air damping include the utilization of perforations in the proof mass and vacuum packaging. Unfortunately, unless a device is packaged in an ultrahigh vacuum environment, air damping can still be a significant dissipation source contributing to a deterioration in the quality factor. In an experiment conducted on a polysilicon microbeam resonator, the measured quality factor was found to be a strong function of pressure ranging from the atmospheric pressure down to a few pascals.²⁶ A recent measurement of the quality factor of a gold microplate resonator indicates that air damping is a dominant factor even when the ambient pressure is as low as 100 Pa.²⁷

Air damping, i.e., the damping force exerted on moving microresonators, is dictated by gas transport and its interaction with the resonator. In a rarefied gas, which can be caused either by low pressure or by small characteristic length, the collision between gas molecules and resonators is an important if not a dominant factor in determining the flow behavior. The level of gas rarefaction can be characterized by the Knudsen number (Kn), defined as the ratio between the molecular mean free path and the characteristic length. When the Knudsen number is 10 and up, gas becomes so rarefied that intermolecular collisions rarely occur and hence their effect on gas transport can be neglected. Such a flow is called free-molecule flow and the corresponding gas regime ($\text{Kn} \geq 10$) is the free-molecule regime. For resonators packaged in a low vacuum, the free-molecule regime is often

encountered. For example, if a resonator with a characteristic length of a few microns oscillates inside a vacuum with a pressure of a few pascals, the Knudsen number of the gas surrounding the resonator is on the order of 100. In the free-molecule regime, continuum theories built upon the assumption that intermolecular collisions dominate gas transport break down and methods/models based on these theories are no longer applicable.

Air damping has been modeled extensively by many researchers. When air is in the continuum regime, Reynolds' equation is often employed to predict the squeeze-film damping between two plates with a thin gap.^{1–3,5,10,11} Extension of this approach to perforated plates has also been made.⁷ When the gap is not too thin, Reynolds' equation is no longer accurate. Numerical simulations of the Navier–Stokes equations have been conducted to model squeeze-film damping^{4,9} in such cases and system-level damping models have been extracted based on numerical simulations.^{6,8}

For rarefied air damping, the modeling approaches can be classified into two main categories. One is based on the modification of continuum theories. Examples in this category include, but are not limited to, the modification of Reynolds' equation by employing the effective viscosity obtained either from a linearized Bhatnagar–Gross–Krook solution of the Poiseuille flow^{12,14,23} or from experimental data^{24,25} via curve fitting, by using a pressure dependent effective flow rate coefficient¹³ and a modified pressure boundary condition with coefficients extracted from the Navier–Stokes slip-jump simulations and the direct simulation Monte Carlo (MC) simulations.¹⁵ Most of these methods have demonstrated their accuracy in the slip regime ($\text{Kn} \leq 0.1$), i.e., the near continuum regime. The applicability of most of these methods in the free-molecule regime is, however, theoretically questionable.²⁸

Another type of approach is based on individual molecule transport. In the free-molecule regime, Christian¹⁶ de-

veloped an elegant analytical model for the quality factor of an isolated solid structure oscillating rigidly in a gas in 1967. This model was later employed in the modeling of several microresonators despite the fact that in some cases, the oscillating structure was close to a stationary wall. A recent work has extended the Christian model to cantilevers, bridges, and torsional resonators.²¹ All of these oscillate in an unbounded gas. The importance of a nearby fixed wall, representing either a substrate or an electrode in many cases, was first recognized by Bao *et al.*,¹⁷ who employed an elastic-collision model to calculate gas damping. In order to derive a close-form expression for the quality factor, several assumptions were employed in Bao's model. Unfortunately some of these assumptions are quite critical to the accuracy of the prediction. A semimolecular approach which tracks the motion of a representative particle and its collisions with oscillating resonator was proposed¹⁸ to quantitatively evaluate these assumptions. It was found that some of the assumptions employed in Bao's model could lead to more than a 50% underprediction of air damping. Although the semimolecular approach has brought the prediction of air damping of Zook's resonator²⁶ much closer to the experimental data than any other existing molecular based approaches, 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 molecular simulation would improve the accuracy greatly. However, the major drawback of such a method is the massive computational power required, which prohibits its use as a practical design tool.

From designer's perspective, a model that correlates the performance of the device directly with device parameters is highly desirable. This paper presents the development of a macromodel which relates air damping explicitly with device parameters such as dimensions, oscillating amplitude and frequency, and initial gap between the resonator and the fixed wall. This model is built upon statistical theory and full molecular simulations to ensure its accuracy. The basic assumptions employed in the model are (1) elastic collisions between gas molecules and resonators, (2) rigid motion of resonators, and (3) rectangular plate resonators. The extension to a more general situation is discussed in Sec. V.

II. MC SIMULATION

The resonators considered are of parallel-plate type. The top plate represents the resonant structure while the bottom plate represents the fixed substrate which often acts as an electrode. Let the origin of a Cartesian coordinate system be at the bottom plate and the oscillation direction be along the x axis [Fig. 1(a)]. The position of the top plate is then described by $x = d - A \sin \omega u$, where d is the initial gap between the top plate and the fixed substrate and A and ω are the oscillation amplitude and angular frequency, respectively. The length, width, and thickness of the top plate are denoted as a , b , and h , respectively. As the plate moves up and down, the gas inside the gap is squeezed in and out. As a result, a damping force is produced which dissipates the resonator's energy. The amount of the energy loss can be quantified by

FIG. 1. (Color online) Schematics of the parallel-plate resonator (a) and the corresponding molecular simulation domain (b).

the quality factor Q defined as the ratio of the total input energy to the dissipated energy per cycle.

In order to develop an accurate and general approach for calculating the energy loss of the resonator, a three-dimensional molecular 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 in 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, while the change in the normal velocity v_x satisfies the conservation equations as follows:

$$mv_x + MV = m\tilde{v}_x + M\tilde{V}, \quad (1)$$

$$mv_x^2 + MV^2 = m\tilde{v}_x^2 + M\tilde{V}^2, \quad (2)$$

where m and M are the masses of a gas molecule and the resonator, respectively, v_x and $\tilde{v}_x$ are the pre- and postcollision normal velocities of the gas molecule, and V and $\tilde{V}$ are pre- and postcollision normal velocities of the resonator. Taking into account the extremely small mass ratio between a gas molecule and the resonator, the postcollision normal velocity of the gas molecule is obtained from Eqs. (1) and (2) as

$$\tilde{v}_x = 2V - v_x. \quad (3)$$

In a head-on collision event, a gas molecule gains a velocity of $2|V|$. In a head-tail collision event, it loses or gains a velocity of $2|V|$, depending on the relative speed of the gas molecule and the resonator.

Figure 1(b) illustrates the computational domain of the molecular simulation. 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 the plates, they leave the interaction region without being reintroduced on the opposite side. This allows the finite-size effect of the device to be modeled. To improve efficiency, a surface generation algorithm is employed.²⁹ Molecules are emitted into the interaction region from its open boundary at a rate that is determined by the gas density and temperature at the surrounding reservoir. Their initial positions are uniformly distributed along the boundary. The normal velocity of these molecules is generated based on the one-sided Maxwell-Boltzmann velocity distribution and their tangential components are generated based on the

Maxwell–Boltzmann distribution.³⁰ This molecular approach is similar to the test particle MC method. Hence it is referred as the MC method throughout the rest of this paper.

The outline of the MC algorithm is as follows. At the beginning of the first cycle, gas molecules inside the interaction domain are initialized assuming the system is at equilibrium. Each oscillation cycle of the resonator is then discretized into many small time intervals. At the beginning of each time interval, molecules that will enter the interaction domain within this time interval are generated using the surface generation algorithm. It should be pointed out that within each time interval, molecules enter the domain continuously throughout the interval. Hence by generating molecules all at once at the beginning of each time interval is an approximation. However, this approximation does not produce large errors if the time interval is chosen to be sufficiently small. The newly entered molecules, together with the existing ones, are advanced for one time step following their velocities. A check for possible collisions is then conducted for each molecule. This is done by comparing the x -coordinates of the gas molecules and the oscillation plate. If a collision is detected, the velocities of the gas molecules that collide with the plate are modified according to Eq. (3) and changes in the molecular kinetic energy are recorded and stored. Molecules that leave the interaction domain during this time interval are discarded. This procedure is repeated until the whole period ends. The total energy loss per cycle is then simply the summation of all the changes in the molecular kinetic energy during that cycle. The number of cycles simulated is determined by the convergence of the energy loss. In addition, ensemble averaging is also performed and the convergent value is employed to calculate the quality factor.

III. MACROMODEL

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, i.e., the traveling time, and energy exchange between molecules and the resonator at each collision. Although gas molecules enter the interaction domain with different velocities and from various locations, it is possible to employ a density function to describe the traveling-time distribution and derive an expression of energy loss in terms of the distribution function.

Consider a cycle at which the system (resonator and gas) has reached its quasisteady state and denote it as the N th cycle. The energy loss of the resonator within this cycle, $\Delta E^{(N)}$, consists of two parts. The first part, denoted as $\Delta E_1^{(N)}$, comes from the collisions with molecules that enter the interaction domain within this cycle, and the second part, denoted as $\Delta E_2^{(N)}$, comes from the collisions with those molecules that are initially inside the interaction domain. These molecules either entered the interaction domain within the previous cycle or are already inside the domain at the beginning of the previous cycle. Hence, $\Delta E_2^{(N)}$ again has two components, $\Delta E_2^{(N)} = \Delta E_1^{(N-1)} + \Delta E_2^{(N-1)}$, with $\Delta E_1^{(N-1)}$ being the energy change contributed from molecules entering the do-

main within the $(N-1)$ th cycle and $\Delta E_2^{(N-1)}$ being the energy change contributed from molecules that are initially inside the domain. This process continues and one can conclude that

$$\Delta E^{(N)} = \Delta E_1^{(N)} + \Delta E_1^{(N-1)} + \cdots + \Delta E_1^{(1)} + \Delta E_2^{(1)}. \quad (4)$$

If N is large, the fraction of molecules whose traveling times are equal to or are longer than N periods is extremely small (see Sec. IV). Hence, the energy loss within the N th cycle is mostly due to molecules coming from outside the interaction region, that is,

$$\Delta E^{(N)} = \sum_{j=1}^{j=N} \Delta E_1^{(j)}. \quad (5)$$

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, $\bar{V} = \sqrt{8kT/\pi m}$ 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 these, the number of molecules with traveling times falling within the range of $(t, t+dt)$ is $\frac{1}{4}n\bar{V}L(d-A\sin\omega u)f(t)dt$, where $f(t)$ is the normalized probability density function of molecular traveling time t . Let $e_{u,t}$ be the average energy change in molecules entering the domain at time u and interacting with the resonator for a time period of t . The expression of $\Delta E_1^{(N)}$ can be obtained by summing up the contributions of all molecules that enter the interaction domain within the N th period and have traveling times in the range of $(0, \infty)$. It reads

$$\begin{aligned} \Delta E_1^{(N)} = & \int_0^{T_o} \int_0^{T_o-u} \frac{1}{4}n\bar{V}L(d-A\sin\omega u)e_{u,t}f(t)dtdu \\ & + \int_0^{T_o} \int_{T_o-u}^{\infty} \frac{1}{4}n\bar{V}L(d-A\sin\omega u) \\ & \times f(t)dt \cdot e_{u,T_o-u}du, \end{aligned} \quad (6)$$

where T_o is the oscillation period and e_{u,T_o-u} is the average energy change in molecules that have an interaction time with the resonator of T_o-u . The first integral in Eq. (6) gives the energy change in molecules with a traveling time within the range of $[0, T_o-u]$. Those molecules fly out of the interaction domain before the end of the N th period. The second integral gives the energy change in molecules remaining inside the interaction domain after the N th period ends, i.e., those with a traveling time longer than T_o-u . Since only air damping within the N th period is considered, the average energy change associated with these molecules within the N th period is e_{u,T_o-u} . To derive $\Delta E_1^{(N-1)}$, one must realize that only molecules with a traveling time longer than T_o-u can contribute to the energy loss within the N th period (Fig. 2). Hence, $\Delta E_1^{(N-1)}$ is

FIG. 2. (Color online) Illustration of time periods.

$$\begin{aligned} \Delta E_1^{(N-1)} = & \int_0^{T_0} \int_{T_0-u}^{2T_0-u} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times [e_{u,t} - e_{u,T_0-u}] f(t) dt du \\ & + \int_0^{T_0} \int_{2T_0-u}^{\infty} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times f(t) dt \cdot [e_{u,2T_0-u} - e_{u,T_0-u}] du. \end{aligned} \quad (7)$$

Similarly, one can show

$$\begin{aligned} \Delta E_1^{(j)} = & \int_0^{T_0} \int_{(N-j)T_0-u}^{(N+1-j)T_0-u} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times [e_{u,t} - e_{u,(N-j)T_0-u}] f(t) dt du \\ & + \int_0^{T_0} \int_{(N+1-j)T_0-u}^{\infty} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times f(t) dt \cdot [e_{u,(N+1-j)T_0-u} - e_{u,(N-j)T_0-u}] du, \end{aligned} \quad (8)$$

$j = N-1, N-2, \dots, 2, 1.$

The summation of $\Delta E_1^{(j)}$ over index j yields

$$\begin{aligned} \sum_{j=1}^{j=N-1} \Delta E_1^{(j)} = & \int_0^{T_0} \int_{T_0-u}^{NT_0-u} \frac{1}{4} n \bar{V} L \\ & \times (d - A \sin \omega u) e_{u,t} f(t) dt du \\ & + \int_0^{T_0} \int_{NT_0-u}^{\infty} \frac{1}{4} n \bar{V} L \\ & \times (d - A \sin \omega u) e_{u,NT_0-u} f(t) dt du \\ & + \int_0^{T_0} \int_{T_0-u}^{\infty} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times e_{u,T_0-u} f(t) dt du. \end{aligned} \quad (9)$$

Substituting Eqs. (6) and (9) into Eq. (5), the total energy loss within the N th cycle is obtained as

$$\begin{aligned} \Delta E^{(N)} = & \int_0^{T_0} \int_0^{NT_0-u} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) e_{u,t} f(t) dt du \\ & + \int_0^{T_0} \int_{NT_0-u}^{\infty} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) \\ & \times e_{u,NT_0-u} f(t) dt du. \end{aligned} \quad (10)$$

Based on the fact that when N is large, the fraction of molecules with traveling times larger than $NT_0 - u$ is very small

FIG. 3. (Color online) The top view of a rectangular plate resonator with a gas molecule sitting at the entrance.

(verification is shown in Sec. IV), Eq. (10) can be further simplified as follows:

$$\Delta E^{(N)} = \int_0^{T_0} \int_0^{NT_0} \frac{1}{4} n \bar{V} L (d - A \sin \omega u) e_{u,t} f(t) dt du. \quad (11)$$

Note that in Eq. (11), the interaction time t can be larger than T_0 . This is due to the contributions of the molecules that enter the interaction domain before the N th period.

Exchanging the integration order and letting $\Delta \bar{E}_t = (2\pi/kT/2) \int_0^{T_0} (1/T_0) [1 - (A/d) \sin \omega u] e_{u,t} du$ be the normalized average energy change in molecules with an interaction time of t , the total energy loss of one cycle can then be expressed as

$$\Delta E^{(N)} = \frac{1}{4} n \bar{V} L d T_0 \frac{kT}{4\pi} \int_0^{NT_0} \Delta \bar{E}_t f(t) dt. \quad (12)$$

For the rectangular plate resonators, the traveling-time distribution can be derived analytically. The expression for $\Delta \bar{E}_t$ is difficult, if not impossible, to derive analytically. In this work, it is found via MC simulations.

A. Probability density function of molecular traveling time

Due to elastic collisions, the in-plane velocities of a gas molecule, i.e., V_y and V_z , remain constant during its interaction with the resonator. Hence, the traveling time of each molecule is determined solely by its initial in-plane velocity and its initial in-plane location. Figure 3 shows the top view of a rectangular resonator with lateral dimensions denoted as a and b . Without losing generality, it is assumed that $b \geq a$. Because of the uniform distribution of the initial locations of gas molecules along the perimeter and the symmetric in-plane velocity distribution about the normal direction of the perimeter, only molecules located on the bottom and right edges and with $\theta \in [0, \pi/2]$, where θ is the polar angle of the in-plane velocity, are considered.

FIG. 4. Domain of random variables (U, W) . FIG. 5. Domain of $G(l/v \leq t)$.

1. Traveling distance distribution

Let Ω_A , Ω_B , and Ω be the sample spaces of the traveling distance for molecules located on the bottom edge, molecules located on the right edge, and all molecules, respectively. L , L_A , and L_B are the traveling distance variables defined in Ω , Ω_A , and Ω_B . The probability density function of L is

$$f_L(l) = P_A f_{L_A}(l) + P_B f_{L_B}(l), \quad (13)$$

where l denotes a particular value that L , L_A , and L_B may assume that, P_A and P_B are the probabilities of molecules located on the bottom edge and on the right edge, respectively. Due to the uniform distribution of molecular location, these probabilities are found to be

$$P_A = \frac{1}{1 + \gamma}, \quad P_B = \frac{\gamma}{1 + \gamma}, \quad (14)$$

where $\gamma = b/a$. Equation (13) thus becomes

$$f_L(l) = \frac{1}{1 + \gamma} f_{L_A}(l) + \frac{\gamma}{1 + \gamma} f_{L_B}(l). \quad (15)$$

Defining the nondimensional distance as $L_A^* = L_A/a$, the traveling distance is found to be a function of two independent random variables U and W , defined as $U = 1 - Y/a$ and $W = \cos \Theta$, where Y is the y -coordinate of a molecule at the perimeter and Θ is the polar angle of the in-plane velocity,

$$L_A^* = \begin{cases} \frac{U}{W}, & \frac{U}{\sqrt{\gamma^2 + U^2}} \leq W \leq 1, \\ \frac{\gamma}{\sqrt{1 - W^2}}, & 0 \leq W \leq \frac{U}{\sqrt{\gamma^2 + U^2}}. \end{cases} \quad (16)$$

The distribution of U is uniform. Its density function is thus $f_U(u) = 1$, $0 \leq u \leq 1$. The probability density function of Θ is $f_\Theta(\theta) = \sin \theta$, $0 \leq \theta \leq \pi/2$, which implies that the distribution of W is also uniform, i.e., $f_W(w) = 1$, $0 \leq w \leq 1$.³¹ This leads to a uniform joint density $f_{U,W}(u, w) = f_U(u) \cdot f_W(w) = 1$, $0 \leq u, w \leq 1$.

Figure 4 illustrates the domain of (U, W) . Due to the different relationships between L_A^* and U and W in the two regions Ω_1 and Ω_2 , the probability density of L_A^* has to be found by finding the density functions of the traveling distance in the two regions separately, i.e.,

$$f_{L_A^*}(l) = f_{L_{A1}^*}(l) P_{\Omega_1} + f_{L_{A2}^*}(l) P_{\Omega_2}, \quad (17)$$

where P_{Ω_1} and P_{Ω_2} are the probabilities of a molecule with U and W values within Ω_1 and Ω_2 , respectively. It is not difficult to find that $P_{\Omega_1} = 1 + \gamma - \sqrt{1 + \gamma^2}$ and $P_{\Omega_2} = \sqrt{1 + \gamma^2} - \gamma$ due to the uniform distribution of both U and W . Also the joint density functions of U and W in region Ω_1 and region Ω_2 are $f_{(U,W) \in \Omega_1}(u, w) = 1/(1 + \gamma - \sqrt{1 + \gamma^2})$ and $f_{(U,W) \in \Omega_2}(u, w) = 1/(\sqrt{1 + \gamma^2} - \gamma)$, respectively.

The cumulative distribution function of the traveling distance on Ω_1 can then be derived as

$$\begin{aligned} F_{L_{A1}^*}(l) &= P(L_{A1}^* \leq l) = P\left(\frac{U}{W} \leq l\right) = \int \int_{u/w \leq l} f_{(U,W) \in \Omega_1}(u, w) du dw = \frac{1}{1 + \gamma - \sqrt{1 + \gamma^2}} \int \int_{u/w \leq l} du dw \\ &= \frac{1}{1 + \gamma - \sqrt{1 + \gamma^2}} \begin{cases} \frac{l}{2}, & 0 < l \leq 1, \\ \frac{1}{2} \left(1 - \frac{1}{l}\right), & 1 < l \leq \gamma, \\ \frac{1}{2\gamma} + \gamma - \frac{1 + \gamma^2}{2l} - \frac{l}{2}, & \gamma < l \leq \sqrt{1 + \gamma^2}. \end{cases} \end{aligned} \quad (18)$$

The derivative of $F_{L_{A1}^*}(l)$ with respect to l yields the expression of the probability density function of the traveling distance in Ω_1 as shown in Eq. (19),

$$f_{L_{A1}}^*(l) = F_{L_{A1}}'(l) = \frac{1}{1 + \gamma - \sqrt{1 + \gamma^2}} \begin{cases} \frac{1}{2}, & 0 < l \leq 1, \\ \frac{1}{2l^2}, & 1 < l \leq \gamma, \\ \frac{1 + \gamma^2}{2l^2} - \frac{1}{2}, & \gamma < l \leq \sqrt{1 + \gamma^2}. \end{cases} \quad (19)$$

Following the same approach, the probability density function of the traveling distance in Ω_2 can be derived as

$$\begin{aligned} f_{L_{A2}}^*(l) &= F_{L_{A2}}'(l) = \frac{d}{dl} \int \int_{\gamma/\sqrt{1-w^2} \leq l} f_{(U,W) \in \Omega_2}(u,w) du dw \\ &= \frac{d}{dl} \left\{ \frac{1}{(\sqrt{1+\gamma^2} - \gamma)} \left[\int_0^{\sqrt{l^2-\gamma^2}} \int_0^{\sqrt{u^2+\gamma^2}} dw du + \int_{\sqrt{l^2-\gamma^2}}^1 \int_0^{\sqrt{l^2-\gamma^2}/l} dw du \right] \right\} \\ &= \frac{1}{(\sqrt{1+\gamma^2} - \gamma)} \cdot \frac{\gamma^2}{l^2} \left(\frac{1}{\sqrt{l^2-\gamma^2}} - 1 \right), \\ \gamma < l &\leq \sqrt{1+\gamma^2}. \end{aligned} \quad (20)$$

Combining the two distributions as in Eq. (17), the probability density function of the traveling distance of molecules initially located at the bottom edge is

$$f_{L_A}^*(l) = \begin{cases} \frac{1}{2}, & 0 < l \leq 1, \\ \frac{1}{2l^2}, & 1 < l \leq \gamma, \\ \frac{1}{l^2} \left[\frac{1 - \gamma^2 - l^2}{2} + \frac{\gamma^2}{l^2} \right], & \gamma < l \leq \sqrt{1 + \gamma^2}. \end{cases} \quad (21)$$

Similarly, the density distribution function of the traveling distance of molecules which enter the interaction domain from the right edge is

$$f_{L_B}^*(l) = \begin{cases} \frac{1}{2\gamma}, & 0 < l \leq 1, \\ \frac{1}{\gamma l^2} \left(\frac{\gamma}{\sqrt{l^2-1}} - \frac{1}{2} \right), & 1 < l \leq \gamma, \\ \frac{1}{\gamma l^2} \left[\frac{\gamma - 1 - l^2}{2} + \frac{\gamma}{\sqrt{l^2-1}} \right], & \gamma < l \leq \sqrt{1 + \gamma^2}. \end{cases} \quad (22)$$

Substituting Eqs. (21) and (22) into Eq. (15), one obtains the density function of the traveling distance as

$$f_L^*(l) = \begin{cases} \frac{1}{1 + \gamma}, & 0 < l \leq 1, \\ \frac{1}{1 + \gamma} \frac{\gamma}{l^2 \sqrt{l^2-1}}, & 1 < l \leq \gamma, \\ \frac{1}{1 + \gamma} \left[\frac{1}{l^2} \left(\frac{\gamma^2}{\sqrt{l^2-\gamma^2}} + \frac{\gamma}{\sqrt{l^2-1}} \right) - 1 \right], & \gamma < l \leq \sqrt{1 + \gamma^2}. \end{cases} \quad (23)$$

2. Traveling-time distribution

The traveling time of a gas molecule is the ratio of its traveling distance and its in-plane speed. The in-plane molecular speed (V_{yz}), which is a random variable, has a probability density function of $f_{V_{yz}}(v_{yz}) = \sqrt{2/\pi} (m/kT)^{3/2} \times v_{yz}^2 \cdot e^{-mv_{yz}^2/2kT}$, $0 \leq v_{yz} < +\infty$, where m is the molecular mass, k is the Boltzmann constant, T is the temperature, and v_{yz} denotes a particular value that V_{yz} may assume. Let $V^* = V_{yz}/c$ be the nondimensional in-plane speed, where $c = \sqrt{kT/m}$. The density function in the nondimensional form is

$$f_{V^*}(v) = c \cdot f_{V_{yz}}(cv) = \sqrt{\frac{2}{\pi}} v^2 \cdot e^{-v^2/2}, \quad 0 \leq v < +\infty. \quad (24)$$

With the probability density functions of both traveling distance and speed, the cumulative distribution function of the

nondimensional traveling time, defined as $T_t^* = L^*/V^*$, can be deduced as

$$F_{T_t^*}(t) = P(T_t^* \leq t) = \int \int_{l/v \leq t} f_{L^*, V^*}(l, v) dl dv = \int \int_G f_{L^*, V^*}(l, v) dl dv, \quad (25)$$

where the domain G is illustrated in Fig. 5.

Since traveling distance and speed are independent of each other, their joint density function is simply the product of the individual density functions. The cumulative distribution function of traveling time is thus

$$\begin{aligned} F_{T_t^*}(t) &= \int \int_G f_{L^*}(l) \cdot f_{V^*}(v) dl dv \\ &= \int_0^{1/t} \int_0^{t \cdot v} f_{L^*}(v) \cdot f_{V^*}(v) dl dv + \int_{1/t}^{\infty} \int_0^1 f_{L^*}(v) \cdot f_{V^*}(v) dl dv + \int_{1/t}^{\gamma/t} \int_1^{t \cdot v} f_{L^*}(v) \cdot f_{V^*}(v) dl dv \\ &\quad + \int_{\gamma/t}^{\infty} \int_1^{\gamma} f_{L^*}(v) \cdot f_{V^*}(v) dl dv + \int_{\gamma/t}^{\sqrt{\gamma^2+1}/t} \int_0^{t \cdot v} f_{L^*}(v) \cdot f_{V^*}(v) dl dv + \int_{\sqrt{\gamma^2+1}/t}^{\infty} \int_{\gamma}^{\sqrt{\gamma^2+1}} f_{L^*}(v) \cdot f_{V^*}(v) dl dv \\ &= \frac{1}{1+\gamma} \left[1 + \gamma + (1 - e^{-\gamma^2/2t^2}) \left[\sqrt{\frac{2}{\pi}} t (1 - e^{-\gamma^2/2t^2}) - \gamma \operatorname{Erf}\left(\frac{\gamma}{\sqrt{2}t}\right) \right] \right] + (1 - e^{-1/2t^2}) \left[\sqrt{\frac{2}{\pi}} t (1 - e^{-1/2t^2}) - \operatorname{Erf}\left(\frac{1}{\sqrt{2}t}\right) \right] \Bigg|_0 \\ &\leq t < \infty. \end{aligned} \quad (26)$$

The derivative of $F_{T_t^*}(t)$ with respect to t yields the density function of traveling time,

$$\begin{aligned} f_{T_t^*}(t) &= \frac{1}{1+\gamma} \left[-\frac{e^{-1/2t^2}}{t^3} \left[\sqrt{\frac{2}{\pi}} t (1 - e^{-\gamma^2/2t^2}) \right. \right. \\ &\quad \left. \left. - \gamma \operatorname{Erf}\left(\frac{\gamma}{\sqrt{2}t}\right) \right] + 2 \sqrt{\frac{2}{\pi}} (1 - e^{-\gamma^2/2t^2}) (1 - e^{-1/2t^2}) \right. \\ &\quad \left. - \frac{\gamma^2 e^{-\gamma^2/2t^2}}{t^3} \left[\sqrt{\frac{2}{\pi}} t (1 - e^{-1/2t^2}) \right. \right. \\ &\quad \left. \left. - \operatorname{Erf}\left(\frac{1}{\sqrt{2}t}\right) \right] \right], \quad 0 \leq t < +\infty. \end{aligned} \quad (27)$$

B. Normalized average energy change of molecules with traveling time of t : $\Delta \bar{E}_t$

1. Key nondimensional parameters

The first task in the derivation of an analytical expression of $\Delta \bar{E}_t$ is to identify the key nondimensional parameters.

Of all the important parameters, resonator dimensions a and b affect only the traveling time and their effect on air damping is thus implicitly included in the traveling time t . The rest of parameters, oscillation amplitude A , angular frequency ω , the initial gap d , and traveling time t , are grouped into two nondimensional parameters as $r = A/d$ and $\tau = \omega t$, where r represents the relative volume change in the interaction domain due to plate motion and τ characterizes the interaction time between gas molecules and the resonator. It was found through MC simulations that such two nondimensional parameters completely characterize $\Delta \bar{E}_t$. Figure 6(a) shows $\Delta \bar{E}_t$, obtained from MC simulations, as a function of t at three different oscillation frequencies: $f_1 = 550$ KHz, $f_2 = 275$ KHz, and $f_3 = 137.5$ KHz. The amplitude and the initial gap in the simulations are set to be $A = 0.11 \mu\text{m}$ and $d = 1.1 \mu\text{m}$, respectively. From the plot one can observe that first $\Delta \bar{E}_t$ is a periodic function of t with its period being the oscillation period, and second the shapes of $\Delta \bar{E}_t$ at different frequencies are similar. It is not difficult to realize that the three curves shown in Fig. 6(a) can be collapsed into one, simply by scaling the traveling time with the oscillation fre-

FIG. 6. (Color online) Dependence of $\Delta\bar{E}_t$ on t (a) and τ (b) at different oscillation frequencies.

quency as shown in Fig. 6(b). This fact indicates $\Delta\bar{E}_t$ depends only on τ , not separately on ω and t . In the remaining test, $\Delta\bar{E}_t$ will be denoted as $\Delta\bar{E}$.

To verify that r indeed is a suitable nondimensional parameter for $\Delta\bar{E}$, several cases with different combinations of A and d have been designed and some are listed in Table I. Figure 7 shows $\Delta\bar{E}$ as a function of τ for different cases. The sole dependence of $\Delta\bar{E}$ on r is clearly demonstrated in the figure.

It should be pointed out that additional validation has been done on many other cases with various parameters selected within the ranges presented in Table II. For a concise presentation, the results corresponding to these cases are not presented in this paper.

2. Curve-fitting formula

To find an appropriate form for $\Delta\bar{E}$, the main features of $\Delta\bar{E}$ are examined. As illustrated in Fig. 7, first, $\Delta\bar{E}$ is a periodic function of τ with a period of 2π . Second, the amplitude of $\Delta\bar{E}$ increases with the increasing r and is close to r^2 when r is small. Lastly, the shape of $\Delta\bar{E}$ follows that of $\sin^2(\tau/2)$. These features suggest that $\Delta\bar{E}$ should possess a form of $r^2 \sin^2(\tau/2) \cdot y(r, \tau)$, where $y(r, \tau)$ is a function to be determined. Further study of the relationships between y and r and τ (Fig. 8) indicates that a proper function form for y is

$$y(r, \tau) = P_0 + \alpha(r) \sin^2 \frac{\tau}{2} + \beta(r) [\tau - (2k+1)\pi]^2, \quad (28)$$

$$2k\pi \leq \tau \leq 2(k+1)\pi, \quad k=0, 1, 2, \dots$$

To determine P_0 , $\alpha(r)$, $\beta(r)$, the peak and the valley of y shown in Fig. 8, i.e., the y values at $\tau=\pi$ and $\tau=2\pi$, are plotted as a function of r (Fig. 9). The visible scatter in y at $\tau=2\pi$ is caused in part by the smaller samples at $\tau=2\pi$ as fewer molecules have longer traveling time. It is also caused by the numerical errors associated with the calculation of y which is equal to $\Delta\bar{E}/[r^2 \sin^2(\tau/2)]$. At $\tau=2\pi$, both $\Delta\bar{E}$ and $r^2 \sin^2(\tau/2) \cdot y(r, \tau)$ are very small, close to zero.

The least-squares fitting of these data yields

$$P_0 = 37.37,$$

$$\alpha(r) = P_0 [\exp(2.115r^2 - 0.089r) - 1], \quad (29)$$

$$\beta(r) = P_0 [\exp(0.235r^2 + 0.031r + 0.0068) - 1] / \pi^2.$$

The average energy change in molecules with an interaction time of τ is thus

$$\Delta\bar{E}(r, \tau) = r^2 \sin^2 \frac{\tau}{2} \left\{ P_0 + \alpha(r) \sin^2 \frac{\tau}{2} + \beta(r) \times [\tau - (2k+1)\pi]^2 \right\}, \quad (30)$$

$$2k\pi \leq \tau \leq 2(k+1)\pi, \quad k=0, 1, 2, \dots$$

TABLE I. Parameters for various cases.

Case	r	d (μm)	A (μm)
Case 1-1	0.01	10	0.1
Case 1-2	0.01	15	0.15
Case 2-1	0.05	8	0.4
Case 2-2	0.05	5	0.25
Case 3-1	0.1	9	0.9
Case 3-2	0.1	6	0.6
Case 4-1	0.25	3	0.75
Case 4-2	0.25	4	1
Case 5-1	0.5	1	0.5
Case 5-2	0.5	2	1

IV. VALIDATION

A. MC simulation

A recent experiment conducted by Sumali²⁷ was chosen to validate the developed MC simulation code. In Sumali's experiment, an electrodeposited gold microplate 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 fourfolded beams as shown in Fig. 10. This design allows the plate to move up and down rigidly, making it a perfect test vehicle for theories and simulations based on the rigid-body-motion

FIG. 7. (Color online) $\Delta \bar{E}$ as a function of τ in various cases.

assumption. The geometry of the central plate is approximated as a rectangle plate with dimensions of $a = 154.3 \mu\text{m}$ and $b = 196.2 \mu\text{m}$. These dimensions are chosen to match its area.²⁷ The thickness of the plate is $5.7 \mu\text{m}$ and the initial gap between the plate and the substrate is $4.1 \mu\text{m}$.

Energy changes in gas molecules within one cycle are computed using the MC code at several different ambient pressure levels. Ensemble averaging is performed to reduce variance. Figure 11 shows the energy change as a function of the number of simulation runs. Each point in the plot represents the cumulative ensemble average of the results ob-

tained through previous runs. Clearly the required number of independent runs in order to achieve a convergence increases with the decreased pressure due to the reduced density at low pressures. Nevertheless, as indicated in the plot, convergence is achieved and the convergent results are used to calculate the quality factor as

TABLE II. Ranges of parameters.

Parameter	Unit	Min.	Max.
a	μm	1	5000
b	μm	0.2	200
A	μm	0.002	1
d	μm	0.02	10
f	kHz	10	10^6

FIG. 8. (Color online) Dependence of y on r and τ , $\tau \in [0, 2\pi]$.

FIG. 9. (Color online) Dependence of $y(r, \tau)$ on r at (a) $\tau=\pi$ and (b) $\tau=2\pi$.

$$Q = \frac{\pi M(A\omega)^2}{\Delta E}, \quad (31)$$

where M represents the effective mass of the resonator including both the central plate and fourfold supporting beams²⁷ and ΔE is the energy loss due to air damping. Table III lists the quality factors at three different pressures, together with their products. It is evident that the product of the quality factor and the pressure is a constant which is consistent with the theoretical prediction.

The comparison between the simulated quality factors and the experimental data is demonstrated in Fig. 12. Simulations are performed at an ambient temperature of 295 K. Also shown in the figure are the results obtained from Bao's model and semimolecular simulations. Clearly MC 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. Table IV lists the relative errors of the modeling results as compared with measured data extracted manually from the original figure. It should be pointed out that all the modeling results shown in Fig. 12 contain the squeeze-film damping only, while the experimental data also include gas damping from the top of the moving

FIG. 10. (Color online) Schematic of Sumali's resonator (top view).

plate. This damping, however, is about a two-order magnitude smaller than the squeeze-film damping. Hence, it has negligible effect on the overall damping.

B. Macromodel

The derived analytical expressions for traveling-time distribution and average energy change of molecules with an interaction time of τ , $\Delta \bar{E}$, are benchmarked using MC simulations. Figure 13 shows the density functions of the traveling time for plates with various aspect ratios, ranging from a square plate ($\gamma=1$) to a narrow beam ($\gamma=100$). The agree-

FIG. 11. (Color online) Energy changes within one cycle at three different ambient pressures.

TABLE III. Simulation results corresponding to three different pressures.

P (torr)	Runs	Q	Q^*P (torr)
0.0001	3600	3 955 741	395.6
0.001	360	395 284	395.3
0.01	36	39 492	394.9

ment between the results obtained from the analytical formula and MC simulations is excellent. From the plot, it is observed that the density decays rapidly after $t=a/c$. For a typical value $a=100 \mu\text{m}$, c/a is around 3 MHz, which indicates that the traveling time of the majority of gas molecules is less than one oscillation period. Such a fact verifies the assumption employed in the derivation of the energy loss formula (Sec. III).

Figure 14 plots the relative errors of $\Delta\bar{E}(r, \tau)$ obtained from the fitting formula, Eq. (30), as compared with MC simulation results. Several resonators with different ratios between the amplitude and the initial gap are tested. The maximum errors in all cases are less than 1%, illustrating the accuracy of the fitting formula.

C. Quality factor

With the analytical expressions for $f(t)$ [Eq. (27)] and $\Delta\bar{E}(\tau, r)$ [Eq. (30)], the energy damping of a plate resonator can be evaluated via the numerical integration of Eq. (12). 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 NT_o with $2T_o$ is less than 0.1%.

Table V lists the parameters of several testing resonators. The first two are real devices,^{26,27} for which the measured quality factors are available. The rest three are arbitrarily made up in order to test various combinations of parameters. The products of the quality factor and the ambient pressure obtained from the derived macromodel and MC simulations are listed in Table VI. Also shown are the experimental data for the first two resonators. The agreement between the MC

TABLE IV. Relative error of Q^*P of Sumali's resonator.

	Q^*P (torr)	Relative error (%)
Measurement	366	...
Bao <i>et al.</i> 's model	2376	549
Semimolecular simulation	848	132
MC simulation	387	5.7

results and the macromodel results is excellent. In all cases the relative errors between the two sets of results are less than 1%, indicating that the simple macromodel has faithfully reproduced the MC results for a wide range of plate resonators. The relative errors between the measured data and macromodel results are 3.9% and 5.7%, respectively, much smaller than the errors produced by any other existing model.

V. DISCUSSION

A. Gas-wall interaction model

A phenomenological and yet practically useful model for gas-wall interaction is the Maxwell model.³² This model employs the accommodation coefficient, a parameter in the range of [0,1], to characterize the collisions. When the accommodation coefficient is 0, the collision is elastic, or specular. When it is 1, the collision is diffusive, i.e., the velocity or the temperature of the reflected molecules has been fully adjusted to that of the surface. Very little work has been published on the measurement of the tangential momentum accommodation coefficient (TMAC) of micromachined surfaces. In an experimental study by Arkilic *et al.*,³³ the TMACs for helium, argon, and carbon dioxide in micromachined silicon channels were found to be less than unity, ranging from 0.75 to 0.85. Another study reported values of 0.91 for helium and 0.87 for nitrogen in a glass channel covered by a flat silicon wafer.³⁴ All these measurements were conducted at the atmospheric pressure. In a vacuum environment, the accommodation coefficient is likely to be smaller due to relatively cleaner surfaces. The developed macromodel is based on elastic collisions. Although no ex-

FIG. 12. (Color online) Comparison of different modeling approaches and Sumali's measurement.

FIG. 13. Probability density functions of traveling time for various plates.

FIG. 14. (Color online) Relative errors of $\Delta\bar{E}$.

perimental measurements of the TMAC of resonators in a vacuum environment are available to justify this assumption, the validity of the macromodel has been proven to a certain extent by the two experiments. A study of the effect of the TMAC on air damping has also been conducted using MC simulations. It has been found that the squeeze-film damping on Sumali's device obtained from the diffuse model is about 3.3% higher than the value obtained from the specular model. Further numerical study of Sumali's device indicates that the difference in the air damping predicted from the specular model and the diffusive model is frequency dependent. At high frequencies, the difference is large. Figure 15 plots the quality factors obtained from the two models at different frequencies. The difference in the quality factor increases from 3.3% to 8% when the frequency increases from 16.9 to 50 kHz. Hence if the TMAC is near unity, the macromodel should be used only for resonators with low resonant frequencies.

B. Rigid body motion

Most resonators oscillate at their deformed modes. The effect of the deformed shape on air damping was theoretically studied for a resonator oscillating in unbounded air and no influence was found from the oscillating shape of the resonator.²⁰ In this study, the measurement of the resonator of Zook *et al.*, i.e., the first resonator listed in Table IV, is performed on its deformed shape while the modeling is done based on rigid-plate assumption. The 3.9% error between the two sets of data seems to indicate that the effect of the deformed oscillating mode on squeeze-film damping in this

TABLE V. Parameters of various resonators.

Unit	a (μm)	b (μm)	d (μm)	A (μm)	f kHz	T (K)
Zook <i>et al.</i> 's resonator	40	200	1.1	0.11	550	273
Sumali's resonator	154.3	192.6	4.1	0.1	16.91	273
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 VI. The product of the quality factor and pressure of various resonators.

	Macromodel	MC simulation	Measurement
Zook <i>et al.</i> 's resonator	401	399	386
Sumali's resonator	384	387	366
Resonator No. 3	76 242	75 510	...
Resonator No. 4	2356	2352	...
Resonator No. 5	2575	2554	...

case is not significant, similar to the case studied in Ref. 20. However, a systematic study should be conducted. The present MC approach can be easily extended to modeling air damping on resonators with deformed shapes.

C. Extension to other shapes

The methodology developed in this study is equally applicable to resonators with other shapes such as disks, plates with holes, etc. The only modification that needs to be done is the traveling-time distribution, which can be obtained either through analytical derivation, similar to the one presented in this paper, or by MC simulation and curve fitting.

VI. SUMMARY

Squeeze-film air damping is an important factor that affects the performance of microresonators even when they are packaged in partial vacuum. The prediction of air damping in a vacuum environment is challenged by the breakdown of the classical Navier–Stokes equations because of the rarefaction effect. Based on the gas kinetic theory, a MC simulation approach is developed to simulate air damping by modeling individual molecule transport. Compared with the existing approaches, the MC approach is the most accurate and general method for the prediction of squeeze-film air damping in the free-molecule regime. The efficiency of this method is, however, very low compared with continuum based methods, which limits its application to the design of microresonators. To overcome the MC method's low efficiency while maintaining its accuracy, a macromodel of squeeze-film damping has been developed for plate resonators with a rectangular shape. This model relates air damping directly with device parameters and hence provides an efficient tool for the de-

FIG. 15. (Color online) Quality factor vs frequency at TMAC=0 and TMCA=1. Ambient pressure is 1 torr.

sign of microresonators with high quality factors. The accuracy of the model is validated by both MC simulations and experimental measurements. Very good agreements have been obtained for a wide range of resonators. It should be pointed out that the application scope of the macromodel, due to the assumption of elastic collision, is limited to resonators with a small TMAC and to resonators with low frequencies if the TMAC is near unity.

ACKNOWLEDGMENTS

This publication is based on work supported in part by Award No. SA-C0040/U.K.-C0016, made by King Abdullah University of Science and Technology (KAUST), and in part by Hong Kong Research Grants Council under Competitive Earmarked Research Grant No. 622109. We would like to thank Dr. H. Sumali (Sandia National Laboratories) for providing us the detailed parameters in his experiment.

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