

Optical Nano/Micro A.C. Generator: A Novel Approach

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Abstract

The need for providing power to micro-systems has been there ever since their advent in technology. This paper presents a novel theoretical approach for generating alternating current for microsystems. The approach is based on combining the well known conventional piezoelectric thin film micro-cantilevers combined with optical behavior of azo-benzene. Azo-benzene molecule undergoes cis- to trans-transformation when exposed to certain wavelength of optical spectra. The effect is utilized to show the actuation for a hypothetical set of dimensions assumed for PZT coated micro- and nano-cantilevers, thereby generating an A.C. pulse. The effect of various parameters on design of above system is also explored. Finally, the optimum design parameters are suggested for practical fabrication of such a generator.

Keywords: Micro/Nano Electro-Mechanical Systems (MEMS/NEMS), Plumbum Zirconate Titanate (PZT) coated micro-cantilevers, Optical Switching, Micro/Nano generators.

1 Introduction

In the recent years, MEMS and NEMS have attained extraordinary attention and importance by providing new tools of exploration in the hands of researchers. Micro/Nano electromechanical systems are the devices used in order to create small scale tools, subjected to external stimuli, for performing tasks at micro and nano levels; e.g., electrostatic charge separation, piezoelectric actuation and photon induced stimulation, applied at scales much shorter than visible.

The proposed system aims to find application at various levels, wherein micro-system power supply is a need. Also, it is suggested that if a large battery of units is made to function in synchronization, it can be used to generate power at macro-scale [1], [2].

Since the advent of MEMS concept, micro-cantilevers have been objects of interest for various applications in most of the sensing and actuation utilities. Similar counterparts of

such structures, which have been used quite extensively are micro-simply supported and overhung beams, diaphragms and membranes [3], [4]. Molecular switching, on the similar lines, is not a new concept and has been innovated to various forms, like optical and chemically induced molecular switches, single molecule switches and supra-molecular switches, suggested and applied successfully [2], [3], [5].

This paper presents a novel theoretical approach for generating alternating current for microsystems. The approach is based on combining the well known conventional piezoelectric thin film micro-cantilevers combined with optical behavior of azo-benzene. Azo-benzene molecule undergoes cis- to trans- transformation, when exposed to certain wavelength of optical spectra. The effect is utilized to actuate PZT coated micro-cantilevers, thereby generating an alternating current (A.C.) pulse. The effect of various parameters on design of above system is also explored. Finally, the optimum design parameters are suggested for practical fabrication of such a generator.

I would like to mention at this stage that, as an overview, the usual design approach adopted in simple cantilever mechanics has also been covered in this work in the section regarding design suggestions.

2 Physics of the Problem

Since the problem involves vibration of cantilever, accompanied by an electrostatic type of actuation taking place, the physics of the problem can be divided into following parts in order to get a complete picture of the relevant mechanism:

- (1) Suggested Setup Design (piezoelectric analysis of the system);
- (2) Design Methodology:
 - (i) static analysis of beam system,
 - (ii) dynamic analysis of the same.

2.1 Working Principle

As a matter of observation, the cis- isomer of azo-benzene, on irradiation by a larger wavelength red light beam, polarized parallel to the direction of cis-transition moment, isomerizes back to trans isomer. Again, if trans isomer is

irradiated by a small wavelength blue light beam of the similar polarization, it gets converted to cis; and on conversion to trans-, cis- gets elongated. Due to increase in length, it also shows increased amounts of anisotropy, compared to its cis- counterpart. Also, it has been observed that the exposure to the circularly polarized red light optimizes the reorientation, though not greatly. In case, both blue and red beams are parallel polarized, there are insignificant amounts of improvements observed [5]. This is due to the fact that, under such a condition, cis- azo-benzene does not absorb red beams polarized perpendicular to their axis. This observation has been utilized herein, by connecting the free end of the cantilever to the base substrate by a film/chain of the above stated type. The setup is then illuminated by the selected wavelengths generating two opposite types of polarities at the fixed end output terminals. The alternating current thus generated, has its frequency dependent upon the frequency with which the azo-benzene film is illuminated by the light beams. It's worth noting here that, at increased frequencies of operation, beyond a certain critical value, the film may fail due to fatigue, thus leading to overall system failure.

Furthermore, it is mentionable that the molecular photo induced reorientation usually takes place in fluid systems, such as liquid crystals. However, the same effect can be achieved, in solid matrices, by polarized beams. The reason is cis- trans interchange on exposure. More stable transomers are the elongated derivatives, whereas cis- isomers are bent, photo induced ones, which quickly get converted back to trans isomers on thermal or optical exposure.

Trans- and cis- azo-benzene isomers have their lengths as 1.0 and 0.56 nm, respectively. This dimensional difference reflects in cis- isomers rotating more easily, compared to trans [5].

The major question that still remains, and is the heart of this proposal, is: how the device would work? Therefore, a complete description of the transduction phenomenon taking place can be given in the following manner. In describing this phenomenon, we assume that initially, the quadramolecular chain of azo-benzene molecules is such that all its constituent molecules are in cis- form. This clearly implies that the cantilever, with which this molecular chain is attached at the free end, would be bent downwards, and the upper face of it would be in a state of tension, the lower face being in compression as a result. This is because the cis-form is shorter in length as compared to its trans-counterpart. Hence, all four molecules in cis-form clearly would make it bend downwards. As soon as this chain is exposed to larger wavelength red light beam, photoisomerization occurs, converting cis- form to trans- form of the azo-benzene molecules. Since each of these molecules gets converted to trans- form, its length increases, as a result of this photo-isomerization, by 0.44 nano-meters. The mean gap height of the cantilever, i.e., the height at which the cantilever would neither be in tension nor in compression at any face, upper or lower, should be assumed to be more than the total length of all four cis-azo-benzene molecules

together, but less than the total length of all the four transomers attached together, end-to-end. Due to this, as soon as the complete cis- to trans- isomerization takes place, the cantilever would certainly be bent upwards. This means that in such a state, the lower face of the cantilever would be in tension, and the upper one, in compression. Therefore, this total change in chain length upon exposure to red light beam changes the sign of stresses on the two faces of the cantilever, and thus that of the piezoelectric layer it carries. This, in turn, assures that a reversal of polarity across the output terminal takes place. This completes one half cycle of the transduction phenomenon. The other half cycle is just the opposite of this, owing to the exposure of the all-trans-azo benzene molecular chain to shorter wavelength blue light beam. This again results into the stress reversal, causing, of course, a polarity reversal just opposite to that observed in the first half cycle. This completes the transduction cycle, which is nothing but a combination of two semi-cycles generating half of an A.C. pulse each.

The continuity of these transduction cycles would result into a continuous A.C. pulse output. The frequency with which this transduction phenomenon is repeated per second determines the frequency of the output A.C. pulse. Fig. (1) shows the two halves of a transduction cycle.

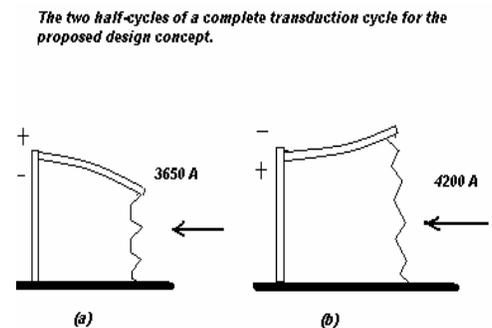


figure 1.a: on exposure to 365 nm light, all cis azo benzene.

figure 1.b: on exposure to 420 nm light, all trans azo benzene.

Figure 1: The schematic showing the proposed design concept. Sub-figures (a) and (b) show the two halves of a complete transduction cycle. 365 nm wavelength converts trans- to cis-, and 420 nm wavelength, cis- to trans.

3 System Analysis and Design

The design and analysis of the proposed system is covered in the following sections.

3.1 Suggested Setup Design (Piezoelectric Analysis)

The setup proposed in this paper is essentially the same as that used in the experimental observations by Baughman et al [6], in order to allow the smooth and correctly oriented

passage of sunlight through the setup. A battery of such units may consist of a number of micro/nano cantilever beams, made up of PZT [Lead Zirconate-Titanate, Pb(Zr,Ti)O₃] deposited over 30x10 (nm)² Au cantilevers, based on a substrate silicon (Si) thick film, such that the faces of all such cantilever beam units are parallel to the substrate film base. The whole set of such cantilevers is similarly oriented, so that the net output has the same nature at all terminals. Also, the whole of the setup is kept inside a 1 molar (1 M) sodium chloride (NaCl) solution, such that the salt solution concentration is uniform throughout. In the later portion of the paper, observations have been made regarding design quality factors, by repeating the same set of calculations, on stainless steel and aluminum cantilevers. Individual cantilever based setups are interconnected at their common output terminals, by electrical connections. The individual cantilevers are essentially thick films of PZT deposited over gold cantilevers, with enhanced ratios of titanium (Ti) included in order to ensure the better strength, as well as natural frequencies of operations, as an instance [7]. Experimental results have shown that increasing PZT thickness and the Ti ratio of the PZT chemistry lead to increased power output for a given deflection [8]. The presence of tensile residual stress in the composite structure can result in lower deflections for a given force and thus impact electrical output. Increasing the Ti ratio leads to a reduction in residual stress. Table 1 shows the various properties of concern regarding different PZT thin film deposited cantilevers.

Table 1: Mechanical properties and residual stresses of films deposited for the cantilever structure. Note that the PZT number indicates the order in which the PZT film was deposited on top of the ZrO₂ layer.

aa	Elastic modulus [GPa]	Poisson ratio	Residual stress [MPa]
PZT1 [12]	63	0.3	630/610
PZT2	63	0.3	-115/-125
PZT3	63	0.3	75/65
PZT4	63	0.3	113/105
ZrO ₂ [13]	244	0.27	400/350
SiO ₂ [14](thermal)	69	0.15	-280/-330
SiO ₂ [14] (PECVD)	69	0.15	35/-15
SiN _x [15]	313	0.29	210/170

The individual cantilevers are connected to their respective bases (substrates) on the free hanging end, by means of a quadra-molecular azo-benzene “spring”, which, in turn, is essentially, a molecular chain consisting of four molecules attached end-to-end with each other.

As another feature, all the 4 molecules are to be kept in the same geometrical isomeric form; viz., all cis- or all trans- so that the molecular chain is at either of the extrema of its possible length. One possible way to keep all the molecules under the same geometrical isomeric states is to keep them at the same temperature, that the cis- form gets converted into trans- form, at slightly elevated temperatures [8]. Also, since the molecular chain is too short in length, and the molecular chain has been considered to be at its extrema of its length, so, the exemplary calculations shown for such a system under the assumed calculation conditions, in fact, provides us with the maximum possible values of the system variables.

The gold cantilever has been selected here as a base for the deposition of PZT films. This comes from the excellent mechanical properties shown by gold under the application conditions for MEMS/NEMS systems. The PZT deposition over this gold cantilever surface may be attained using Physical Vapor Deposition (PVD) or Chemical Vapor Deposition (CVD) techniques, commercially available. Other techniques for similar device fabrication have also been introduced ([7], [9], [10]), which may be opted for.

The polarities generated at the end of the above stated cantilevers may be tapped into circuitry for its power needs using usual arrangements at the fixed end side, as in other conventional micro-generator circuits.

Again, the basic requirement for operating such a generator, i.e., the input energy, comes from typical wavelengths [5]. Since these wavelengths are also present in the atmosphere by virtue of solar radiations on our planet, so it is suggested that we obtain these wavelengths by appropriately filtering them out of the natural solar spectrum available. This forms the basis of differentiation of the suggested devices in that, they can be operated on the naturally available energy input sources, thus making scope for an enormous and efficient harnessing of resources.

3.2 Design Methodology

3.2.1 Static Analysis

In this segment, some of the basic design equations for Radio Frequency MEMS (RF MEMS) operations have been outlined [9], based on which, the calculations of the further sections have been made. Resultant values are based upon the assumed dimensions, which again, as outlined previously, are not realistic, but have been assumed just to explain the concept.

Governing Equation

The governing equation of the system is d'A lamberts' equation. It is assumed that the system to be a non linear, two degree one, thus it should satisfy the following equations:

$$mx'' + bx' + kx = F(\text{ext}) \quad (1)$$

or $\{ ms^2 + bs + k \} X(s) = F(\text{ext})(s) \quad (2)$

Other way round, considering energy conservation for the system,

$$(1/2)(k_1+k_2)*x^2 + (b^2/(2*m))*x^2 = h(v_1+v_2) \quad (3)$$

where x is the bridge displacement, m is the bridge mass, b is the damping coefficient of the system, k is the displacement spring constant and $F(\text{ext})$ is external stimuli. From the values of the corresponding quantities, the value of damping coefficient b was calculated as 10.69, and x was found approximately as 1.76 nm for a quadra-molecular spring of azo-benzene, under the conditions described.

3.2.2 Gas Analysis for the Surrounding Gas/Fluid Environment

In this section, an outline regarding the fluidic environment of the concerned sample MEMS structure has been made, to make the point understandable to the reader..

Mean Free Path of the Fluid Molecules /Atoms

The mean free path of the NaCl ions at 1 atmospheric pressure was estimated as 19.5 μm for Na⁺ ions and 5.5 μm for Cl⁻ ions.

Surrounding atmosphere of the micro cantilever is assumed as 1 molar NaCl solution. This forms the basic fluidic environment of the MEMS structure, the same as noted by Baughman et al.[1]

Knudsen Number

Knudsen number Kn is given in Eq. (4) as,

$$kn = \lambda / g \quad (4)$$

where g is the gap height. The value of gap height for the discussed gold micro cantilever was taken as 3.12 nm, in the order of the dimensions of the cantilever. One major reason for taking it as 3.12 nm is that the gap height must be nearly around the mean length of the minimum and maximum lengths of the azo-benzene chain. This is so as to generate nearly equal deflections in both upper and lower directions, so that equal polarities are generated under both the deflection conditions.

For $g > 1$ nm, $Kn < 0.1$ at STP and the flow may be assumed to be nearly viscous around the setup. So, the problems that may arise out of the viscosity of the surrounding fluid may be neglected by suitably choosing the gap height.

Damping Coefficient / Quality Factor

The damping coefficient is calculated using Eq. (5) as[9]

$$b = 3uxA^2 / (6.28 * g_0^3) \quad (5)$$

Approximate quality factor for the cantilever beam is given in Eq. (6)

$$Q_{\text{cant}} = [E^{0.5} x p x t^2 / (u x w^2 x l^2)] x g_0^3 \quad (6)$$

Also, since the quality is showing strong deviations with gap g_0 , and material constant E , so, again proper combination of material and g_0 is must.

Since damping is a strong function of gap height g_0 , therefore the final value of the quality factor is calculated based on the Sadd & Stiffer expression [4]

$$Q_e = Q [1.1 - (x/g)^2]^{1.5 x} \{ 1 + 9.638 (\wedge/g)^{1.159} \} \quad (7)$$

for a bridge gap g and bridge displacement x in the transverse direction of switching.

The Q_e in this sample calculation was found to be $9.477 \times 10^{-6} \text{Kg}/(\text{m}\cdot\text{s})$. This, indeed, is not a good quality factor value, indicating very poor system quality.

3.2.3 Dynamic Analysis

Dynamic analysis deals with two major parameter determinations: governing force calculations and natural frequency determinations.

For the case of governing force calculations, the governing equation outlined above will be used in the suitable form, so as to get the desired results.

For the case of the natural frequency determinations, we have used the formula in Eq. (8)

$$W(\omega) = k/m \quad (8)$$

knowing that such a system nearly equals a spring mass system. Through numerical simulation techniques, the value of natural frequency of vibration for a $(30 \times 10 \mu\text{m})^2$ thin film was found to be 16.3 kHz[11], having a spring constant value of $2.17 \times 10^{-3} \text{N/m}$, made up of gold..

Another very important parameter, the quality factor was found to be 1.816×10^{-11} , which substantially reflects the importance of design and puts a limitation to size decisions. It is worth mentioning here, that as the quality factor depends drastically upon the gap height of the cantilever, therefore, the quality factor in this case comes out to be so poor. In case we apply greater values of gap heights, then as a consequence, the chain length of azo-benzene will also be needed to be increased, and hence the deflection. In such cases, though, one may have to apply more complex energy balance calculations to get the compensation of factors arising out of the length increase. This is due to the fact that, in order to use longer chains, we may have to

form/encounter thin films of azo-benzene, wherein, the stiffness of the element increases, thus resulting in the said complexities. In such a case, the demonstrative MATLAB coding may also get changed, resulting into different plot results. The changes come due to the reason that, in case of thin films, calculations may involve fixed-fixed beam analysis. In case of molecular chains, one has to obviously apply spring deflection analysis.

Another way, in which the application of optical switching combined to micro-generation set-up may find scope is to measure the stiffness of the thin cantilevers involved. This may be done using the set-up in another way: by applying the wavelengths close to and around the critical values, that actuate the azo-benzene chain and, in the end, to measure the deflections produced. The energy balance equation may then be applied to get the stiffness involved. So, material property measurement may be just another aspect of the same set-up. As the set-up energy balance equation becomes

$$X^2*(Y + c) = d \quad (9)$$

where c and d are known constants, a plot between X and Y can be obtained, using simulative methods. Therefore, for a given set of d and corresponding X, Y can be determined. Here, X & Y denote deflection and stiffness, respectively. c and d can be physically depicted as having dimensions of stiffness and energy respectively.

The energy supplied fundamentally to the generator is that of the light beams which are actually sinusoidal waves. Citing this sinusoidal input applied to the system, we've tried to simulate this system virtually, through MATLAB coding, besides the above shown numerical simulation. The results obtained by this simple simulation technique show the nature of variation of the end loaded cantilever deflection. Also, the frequency response of the system has been shown (in response to the sinusoidal inputs at different frequencies). It is worth mentioning that since the root locus plot of the deflection gives the freedom to chose parameters for the system, as shown in the MATLAB program, we can chose a variety of parametric ways to design such a system, for various applications.

4 Results and Discussions

4.1 Design part

As outlined above, the calculations were made for three possible instances of structures: with gold, aluminium and stainless steel as base cantilever materials, with face dimensions of cantilevers as (10x30) square micro-meters, initially, and then for (10x30) square nano-meters. This change in dimensions has been attributed to improvement in the system quality, denoted by quality factors. The quality factors, for each of them were estimated as 1.81×10^{-2} , 2.02 & 9.74 respectively for the nano dimensions. These values are

better and satisfactory, as compared to those previously calculated. Citing the fact, as outlined above too, that for small (nano-) gap heights but micro-dimensions of the beam, these systems have poor quality, another calculation was made and the quality factor was found to be 1, for a gap height of 2.24 nm, resulting into an improved system, beam dimensions being (10x 30) square nm. This reflects one important fact: the systems have better quality when designed in nano-regime, than when designed in micro-regime. A plot of output displacement versus input energy was also plotted and it was found that the nature of variation is parabolic under this condition. It is worth noting here, that though by considering fluid damping, the system is assumed close to real, but some differences in this nature may arise out of the practical conditions.

The graph in Fig. (2) has been plotted for output transfer function $H(x^2)$ vs. k, the combined stiffness of the (beam + azo-benzene membrane/molecular chain). This figure shows clearly that the deflections decrease sharply with increase in stiffness of the system linearly, i.e., in accordance with the Hook's Law, which has been assumed to be valid for the system. Thus, this observation again confirms the correctness of our approach in the direction.

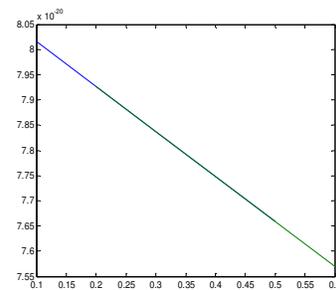


Figure 2: Plot of transfer function vs. combined stiffness(Au)

Roark's formula [11] can be used for the stiffness determination purposes, assuming high speed deflection of cantilevers. The reason for this is that the nature of basic energy equation, used to derive the deflection, is different in this case.

4.2 Matlab-based Behavioral Simulation and Analysis: Interpretations

Referring to the plot in Fig. (3), the system has been simulated for its electro-mechanical actuation part only, and the root locus regarding the system in general has been obtained. As is evident from the plot, since the second root loci shown in green are those corresponding to imaginary roots of the system displacement equation, the system can only be thus "really" fabricable for the range of displacements and natural frequencies obtainable on the third, "real" root line, along the X-axis. As the plot suggests, we can easily opt for a characteristic natural frequency of

vibration chosen from the same, each such frequency corresponding to a typical system gain that can be obtained. As is also shown, the same plot also shows that the damping for such a system is always 1 along the real root line. On similar lines, we can easily choose the system parameters in such a manner that, the damping and roots could be controlled to get a desired system output characteristic. Here, the author would like to point out an important fact: since the system has been modeled on the basis of ideal lines of partition of the input energy, and as the “other” sources of “leakage” of energy have been neglected, the root plot shows the damping effect as a 100% successful process, which, is

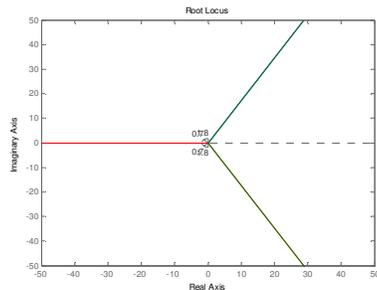


Figure 3: Plot showing design possibility range, based on the root locus of the governing equation.

not “really” so. Therefore, a slight variation in this plot and hence, in the natural characteristics of the designed systems, would occur. The frequency response plot of the same is shown in Fig. (4). Its depictions can be obtained on similar lines for determining the system stability analysis.

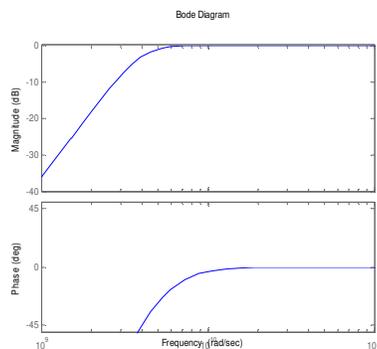


Figure 4: Figure showing the switching times, obtained using the Bode’s plot technique

4.3 Limitations

As the cis form of azobenzene is not thermally stable and a slight warming causes it to return to trans form, optical methods of switching are not for practical use for applications in computing [1]. But since the issue here is not as sensitive as that of optical computing and memory

devices, so, this method may be suggested, with slight modifications in the instrumental setup involved to get the heat removal effect, up to some extent.

Also, it is worth noting that as Azo-benzene is a chemical compound that possesses either of the cis- or trans- forms only, so if we have to generate a bipolar arrangement, we need to keep the mean height of the cantilever as something in between the ‘n’ times of the cis- length or n times of the trans- length. So, the gist is that we need to keep the cantilevers under a state of constant stress. As yet another simple, but important limitation, the formation of NaCl precipitates in non uniform solutions may cause such a system to deviate from its expected behavior. This is attributed to the fact that such systems are very sensitive.

One more point of limitation of the proposed system types is that due to the poor quality, when designed for micro-dimensions. As has been shown in the results and discussions paragraph above, good quality systems in this category require to be designed with macro gap heights, which may not be always appropriate, in the case of a micro-system. Though, the author believes that further focused work in this direction may lead to better quality breakthroughs.

5 Conclusion and Future Work

MEMS/NEMS micro-generators are supposedly a future foundation tool for energy and power-electronics segments. The system outlined in this work is such a one. The design outlines the way it would behave and thus, fulfill its purpose. Better qualities can be assured by choosing correct parameter ranges, as a gist.

The future use of these devices, in the form of large assemblies [1], [2] so as to serve also the macro-power needs of many devices, is suggested.

It is interesting to note that the suggested device, which is actually an optical actuator, can also be utilized for the detection of a certain, though narrow, range of optical wavelengths, falling in vicinity of the noted wavelengths. This behaviour characteristically puts it into the class of optical sensors also. In this case, as can be easily visualized, when the mentioned wavelengths are encountered by the device, it tends to show vibrational outputs, in the form of micro-voltages, which could be realized on any of the modern, high quality micro-voltmeters. Thus, this paves the way for the two way usage of the suggested mechanism, i.e., both as a sensor and an actuator.

(1) The current proposal deals only in terms of theoretical approach being taken on the basis of experimental observations of the major researchers in the field and ,as such , does not deal with any experimentation , at the current level.

(2) The novel approach presented here is under process of work at the Motilal Nehru National Institute of Technology, Allahabad, in order to develop it in full workable forms.

6 References

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Appendix

A Nomenclature

The following nomenclature is used in this paper

λ	Mean free path of the fluid molecules constituting the environment of the setup.
s	Diameter of the gas molecules
N	Number density i.e., fluid density $\rho = N \times m_0$
m_0	Mass of the single molecule
λ_a	Mean free path at the operating pressure: $\lambda_a = (\rho_0 / \rho) \times \lambda$
Kn	Knudsen number = (λ / g)
g	Gap height
μ	Viscosity
R	Specific gas constant
B	Thermal constant for viscosity calculations
μ_e	Viscosity as specified by dependence upon Knudsen number
w	Applied mathematical frequency
Q	Quality factor for the cantilever beam
A	Effective surface area of the cantilever surface
M	Molecular weight of the fluid flowing around the setup