Computational study on ion dynamics of MEMS quadrupole mass filter

B. Anitha, Supriya Gogulapati*, Deepak Kumar Sharma, J. John, M. S. Giridhar, Ashwini Jambhalikar

MEMS Development Division, Laboratory for Electro-Optics Systems (LEOS), ISRO, Bangalore, India

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ABSTRACT

The paper presents the simulation studies for the design of a miniaturized Quadrupole Mass Filter (QMF) based on silicon micromachining technology. Mass spectrometers operating in the range of 1 to 100 amu with the resolution of 1 amu are very useful for science payloads in space missions. The mass filtering action of ions in a filter of length 30 mm with electrodes of radius 250 µm is simulated by standard tools. The complete transmission of ions is examined for various Mathieu parameters which are used to define the operating potentials at the electrodes. The performance parameters namely resolution, mass range and the required design considerations such as initial ion velocity, DC and RF voltages and RF frequency are obtained through the model and the computational program using Mathematica. For the efficient ion transmission, an electrostatic slit with aperture of radius 70 µm is placed before the MEMS QMF. Further, the effects of quadrupole length, focusing voltage and the aperture size on the transmission probability of ions are analyzed.

1. Introduction

Mass spectrometers are the most prominent devices to quantify the composition of gases. They have been widely used in many applications such as space exploration, environmental observation, medical diagnostics, industrial processing etc. The basic mass spectrometer includes an ionizer to ionize the sample, mass filter to quantify the ions of different mass, detector to count the number of emerging ions and the vacuum pump to maintain the system at certain pressure for its operation. It is of great interest to miniature this device which benefits in low cost, light weight, high mechanical and thermal stability, ease in portability, low power consumption and high reliability. Further, the miniaturization will reduce the mean free path of ions and allow the device to operate at higher pressures thereby relaxing the need of large vacuum pumps [1]. Such miniature mass spectrometer can be developed using Micro-Electro Mechanical Systems (MEMS) technology. The advancement of MEMS technology helps to fabricate several mass analyzers concurrently in a single production run. It also offers compatibility to the integration of MEMS devices to associated electronics [2]. The MEMS based mass spectrometers are being studied and reported for its improved performance over the conventional bulk devices [1 - 4]. Based on the principle of filtering action, the mass spectrometers are of different class namely magnetic sector, crossed field, time of flight, quadrupole etc. Among them the Quadrupole Mass Filter (QMF) has emerged as an adaptable appliance owing to its electronically reliant performance [5]. The mass filtering action of QMF with its optimum mass range, transmission and resolution is solely controlled by the applied electric signals. This unique feature makes the device ideal for space flight towards atmospheric studies and environmental monitoring. The prime aim of the authors is to develop MEMS based quadrupole mass spectrometers for space.

*Corresponding author,
E-mail: g_supriya@leos.gov.in

2. Theory of QMF

The QMF is a device that uses the stability of ion trajectories under the applied electric field at the electrodes to separate the ions of specific mass [5]. An ideal QMF has four parallel electrodes of hyperbolic cross section wherein the diagonally opposite electrodes are connected electrically.

One pair of electrodes is connected to a periodic RF potential superimposed on a constant positive DC potential say, $\varphi_x = U + V\cos\omega t$. While, the other is connected to the negative DC voltage and the RF potential of same magnitude as given to the aforesaid electrodes but in opposite phase say, $\varphi_y = -(U + V\cos\omega t)$. Where, U and V are the magnitude of applied DC and RF potentials with ω as the angular frequency of the RF signal. This experimental arrangement will generate a hyperbolic electrostatic field for the mass filtering action. The mathematical relation of the electric potential is given by [3]

$$\varphi(x,y) = \frac{(U + V\cos\omega t)(x^2 - y^2)}{r_0^{\,2}} \quad (1)$$

Here r_0 is the radius of the virtual circle that is drawn tangent to all four electrodes. This inscribed circle will enclose the field effective area between the electrodes for ion transmission.

Using Newton's law following the Laplace equation, the equations of motion of ions moving in such a space temporal potential [3] is given by,

$$\frac{dx^2}{dt^2} + \frac{2e(U + V\cos\omega t)}{mr_0^{\,2}}x = 0 \quad (2)$$

$$\frac{dy^2}{dt^2} - \frac{2e(U + V\cos\omega t)}{mr_0^{\,2}}y = 0 \quad (3)$$

$$\frac{dz^2}{dt^2} = 0 \quad (4)$$

The solutions of above three equations describe the trajectory of ions along the three coordinate axes of the device. It can be seen that the ions that are travelling along z axis are not affected by the potentials applied at the electrodes. They travel freely with the constant axial velocity, $v_z = \sqrt{2eV_z/m}$. Where, '*m*' being the mass of ions and V_z is the accelerating DC potential which are meant to drive ions along the unperturbed z axis. While, the ions moving along the x and y directions are perturbed by the generated hyperbolic field between the electrodes.

The following dimensionless parameters [3,5] can be introduced as

$$\varsigma = \frac{\omega t}{2} \quad (5)$$

$$a_u = \frac{8eU}{mr_0^{\,2}\omega^2} \quad (6)$$

$$q_u = \frac{4eV}{mr_0^{\,2}\omega^2} \quad (7)$$

Here, a_u and q_u are known as Mathieu parameters which contain all the input physical measures for the desired ion transmission in a specified QMF. The subscript 'u' represents the displacement of ions along the x and y axes due to the influence of charged electrodes in a QMF.

The generalized dynamical equation for the ions travelling in a QMF is written as,

$$\frac{d^2u}{d\varsigma^2} + (a_u + 2q_u\cos 2\varsigma)u = 0 \quad (8)$$

This linear second order differential equation is known as *Mathieu equation*. It has a power series solution as a function of Mathieu parameters 'a_u, q_u' with the linear combination of both bounded and unbounded solutions. Only the bounded solutions of Mathieu equation define the stable trajectory of ions. Plots of a_u verses q_u showing the stable and unstable combinations are known as stability diagram and it is depicted in figure 1(a).

From the practical motive, it is desirable to choose the first stability domain which has large values of a_u, q_u points. The enlarged view of the first stability diagram by Mathieu equation is show in the figure 1(b). The operation of QMF can be defined with the help of those a_u and q_u points. Being r_0 fixed for the fabricated QMF, the Mathieu parameters a_u q_u are related to U, V, *m* and ω as in equations (6) and (7). Experimentally, the amplitudes of DC and RF potentials are ramped together to transmit the ions of certain mass. The magnitude of the respective U and V potentials are calculated from the selected values of a_u, q_u and ω. The values of a_u, q_u are selected from the first stability domain to sustain the stability of ions under the applied hyperbolic potential. Simply by tuning the amplitude of U and V, ions of different mass '*m*' are transmitted into the QMF. With this aspect, the QMF is also known as tunable narrow pass band mass filter.

To sustain the resolution of device, it is essential to maintain the ratio of U and V. That is to transmit the ions of different mass, the amplitude of U and V are tuned in such a way that its ratio (U/V)

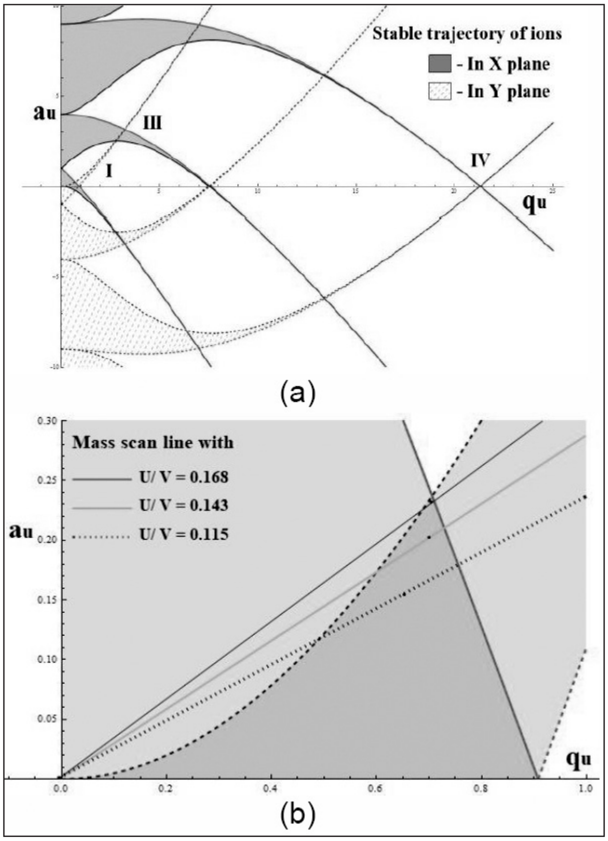

Fig. 1. (a) Stability diagram for the ions in a QMF by Mathieu equation (b) Enlarged view of the first stability domain with three different mass scan lines.

remains constant. The line that drawn from origin to intersect the chosen a_u , q_u points is called mass scan line with slope a/q = 2U/V. The intersection of this mass scan line with the stability diagram will also decide the resolution of QMF. The small portion of such mass scan line with certain mass range will fall in the first stability domain by altering the U/V ratio. When the slope of mass scan line is higher, it results in high resolution. On the other hand, when the slope is lowered by reducing the U/V ratio, the resolution of the device will drop. Besides the value of U/V ratio, the resolution of QMF is experimentally found to depend on the frequency of RF cycle and is defined as [3],

$$\Delta m = \frac{2heV_Z}{f^2L^2} \tag{9}$$

Where, h is the coupling factor between the QMF and ionizer. It typical values are reported to vary from 10 to 20 for the first stability domain [1]. L is the length of quadrupole device and f is the frequency of applied RF signal. The resolving power (R) of the device is given by

$$R = \frac{m}{\Delta m} \approx \frac{n^2}{h} \approx \frac{1}{h}\left(\frac{fL^2}{v_z}\right) \tag{10}$$

Where 'n' is the number of RF cycles experienced by the ions in a QMF.

3. Simulation Results

The 3D simulations on the transmission of ions in MEMS QMF are analyzed using COMSOL 5.2 Multiphysics. As in theory, the model uses the superposition of RF and DC fields for the mass filtering action in a QMF through finite difference method. The model also offers the option to involve the effects of fringing field. For practical concern, the cylindrical electrodes of radius 'r_e' are used in the present simulation. The corresponding best approximation to the ideal hyperbolic field is obtained by fitting the ratio r_e / r_0 =1.148 [3]. The 3D model of simulated MEMS QMF with r_e = 250µm and L = 30 mm is shown in figure 2(a). In the model, the ions are accelerated with an axial energy of 5eV i.e V_z being 5V. Ten ions are released simultaneously with each ion experiencing the DC and the RF potential with the frequency of 6 MHz.

The Mathieu parameters, a_u and q_u are defined in the model as the scaled values for the DC and RF voltages as in equation (5). Which in turn directly relates those operating potentials U and V to r_0^2. Here, the MEMS QMF which has smaller r_e and r_0 will reduce the electrode voltages by double fold. This will enable its operation with less electric field using compact power battery systems. Such advantage of MEMS QMF over the conventional device is presented in figure 2(b) with respect to the RF voltage at the electrodes. As in figure 2(b), to transmit the ions of 40amu, the required RF voltage in BULK QMF say 73V is about 16 times greater than the 4.6 V which is required to transmit the same ions of 40amu in MEMS QMF.

3.1 Analysis of a_u, q_u, parameters

The observed set of a_u, q_u points for the complete ion transmission in the first stability region of Mathieu solution is specified in the plot of figure 3. Since the ions of outer space nearly range from 1-100 amu, the authors are more concerned to transmit those ions using MEMS QMF.

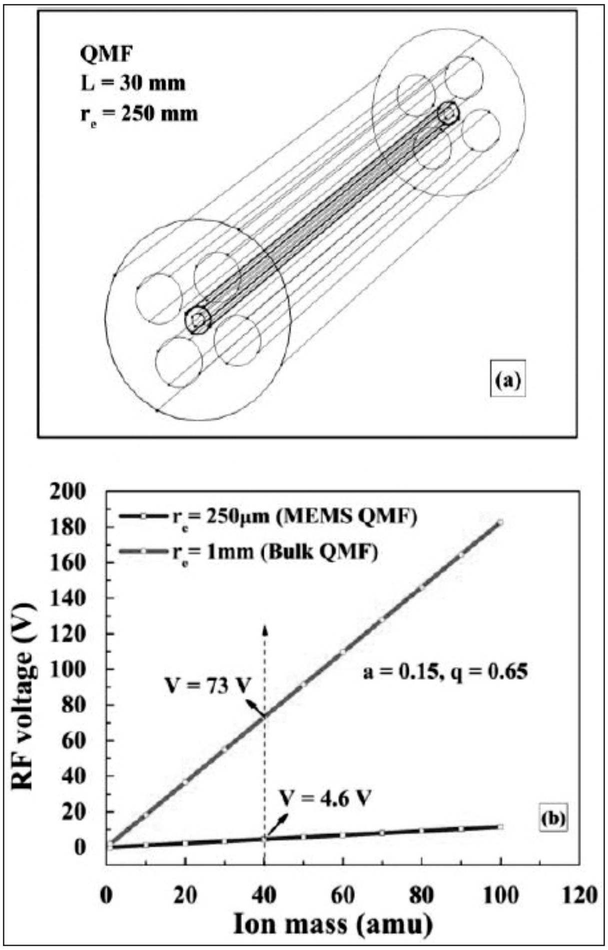

Fig. 2. (a) 3D model of the QMF with inlet path for ions presented in blue lines
(b) RF voltage as a function of ion mass for both MEMS and BULK QMF.

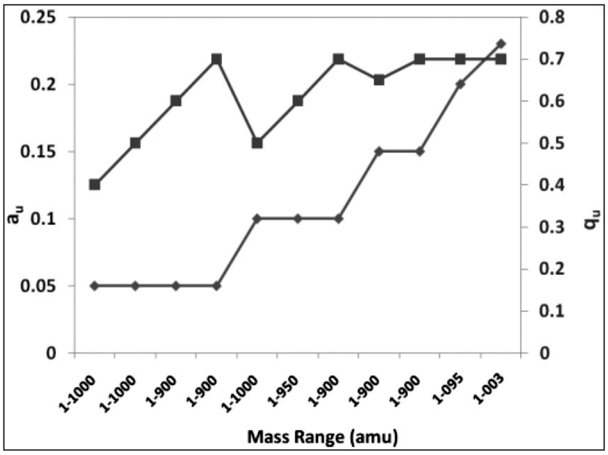

Fig. 3. Set of a_u and q_u values with its mass range for the complete transmission of ion in the considered MEMS QMF.

It has been reported that a_u =0.23 and q_u =0.7 is ideal for a narrow pass band mass filter with high resolution [1-3]. This set of values is found to transmit only few ions of about 1-3amu into the

Table 1
MEMS QMF of different length with its allowable physical parameters.

L (mm)	Mass range (amu)	Resolution Δm (amu)	Resolving Power m/Δm
20	1 - 1000	0.3	1.5 - 1354
30	1 - 900	0.3	3.38 – 2708.8
40	1 – 50	0.17	6 – 300.6
50	1 – 50	0.11	9.39 – 469.7

MEMS QMF which is of not much significance for space exploration. From the above results, it is desirable for the authors to chose only those values of a_u, q_u which have the ion's mass range of about 1-100amu. With respect to resolution which is the main specification for meeting science goals, the rest of the study is simulated for the points a_u = 0.15, q_u = 0.65.

3.2 Effect of the Quadrupole length

When the length of the QMF is reduced by MEMS technique, the flight path of ions will decrease. Therefore, the collision probability of ions will get reduced which enable the device to operate at higher pressure. Further from kinetic theory of gases, the upper limit of pressure is found to vary inversely with device length [3]. This advantage of MEMS QMF will limit the need of heavy vacuum pumps. However, reducing the length less than 20 mm is not recommended because the resolution of the device will drop as in equation 13[2]. For the chosen Mathieu parameters, a_u = 0.15 and q_u = 0.65, the outcome of different physical features by a MEMS QMF of different length is shown in table 1.

As expected, when L increases, the detectable mass range of ions get reduced i.e. the upper limit of ion mass is reduced. This is because the heavy ions which have less kinetic energy are not much affected by the RF field and get discharged at the electrodes for a long flight path. This behavior is verified by the model and its transmission plot for the ion of 100amu with L= 30 and 40 mm are depicted in figure 4. It is observed that all the ions get transmitted completely for L=30 mm. While for L=40 mm, such ions are not transmitted to the detector. The QMF with L = 30 mm is used in the following studies which has the resolution of about 0.3 amu for a_u = 0.15, q_u = 0.65 as referred in Table 1.

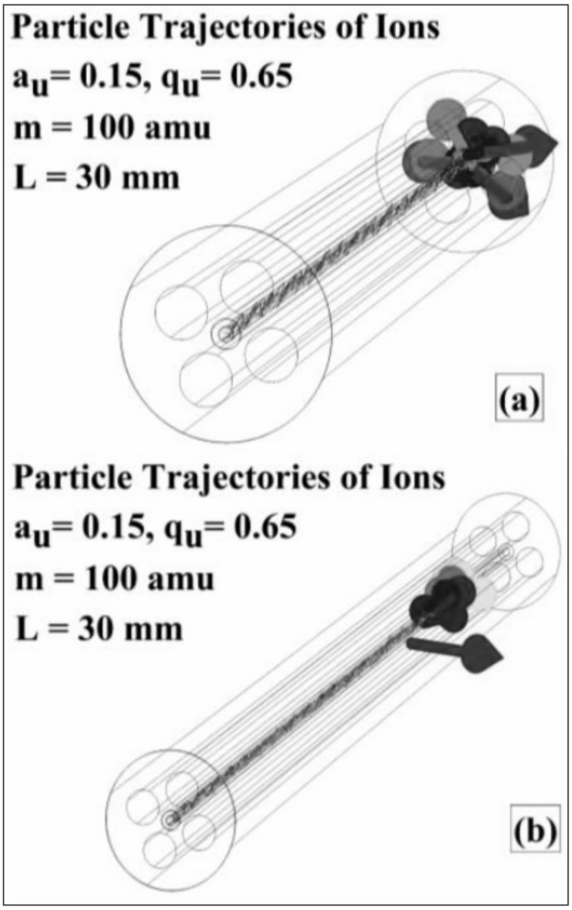

Fig. 4. Transmission of ions in a MEMS QMF with (a) L = 30 mm and (b) 40mm.

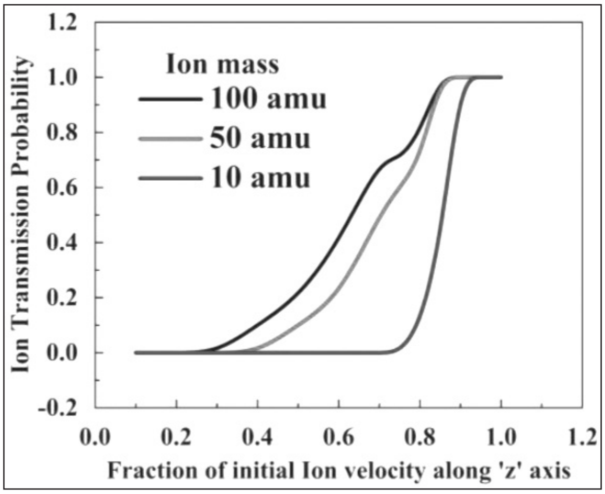

Fig. 5. The transmission probability of ions against the fraction of v_z.

3.3 *Limitation on the initial Ion velocity*

For a given number of ions directed along the axial 'z' direction at voltage V_z = 5V, the transmission possibility of ions with masses 100, 50 and 10amu are presented in figure 5. The transmission probability of ions is found to decrease on increasing the random distribution of ions. When the fraction of $\boldsymbol{v_z}$ is 0.2, only 0.2 $\boldsymbol{v}$ is resolved along the central z axis. So the chance of ions getting transmit out of the device falls down drastically. As well, when the fraction is 1, the ions will have their velocity component completely along the z direction leading to a complete transmission to the detector.

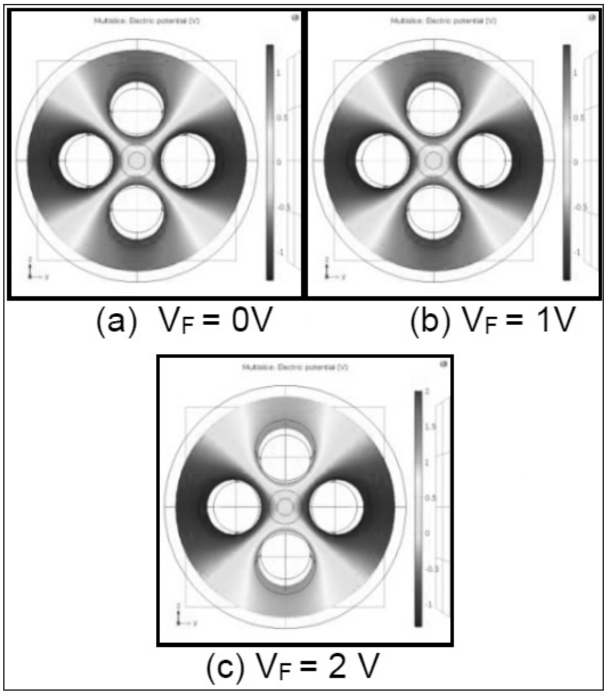

Fig. 6. Effect of focusing voltage on hyperbolic field. The conditions on a_u, q_u is for filtering 100 amu

It is also clear that the heavy ions are less likely to get deviated from the transmission path than the lighter ions. It is because the heavy ions due to its high inertial property manage to transmit the device over the lighter ions. Whereas, the lighter ions which travel with high initial velocity may get discharged at the electrodes in a small interval of time. The possibility of experiencing the quadrupole field for ion transmission is less for the lighter ions at the device entrance. Therefore, the transmission probability of lighter ions drops sharply as the ions are entered more randomly. To overcome this difficulty in real case, it is essential to use the electrostatic lens or slits before the entrance of QMF.

3.4 *Impact of the focusing voltage on the applied hyperbolic potential*

An electrostatic potential is applied to the slit which is just held before the QMF to focus all the incoming ions to the centre of device. As

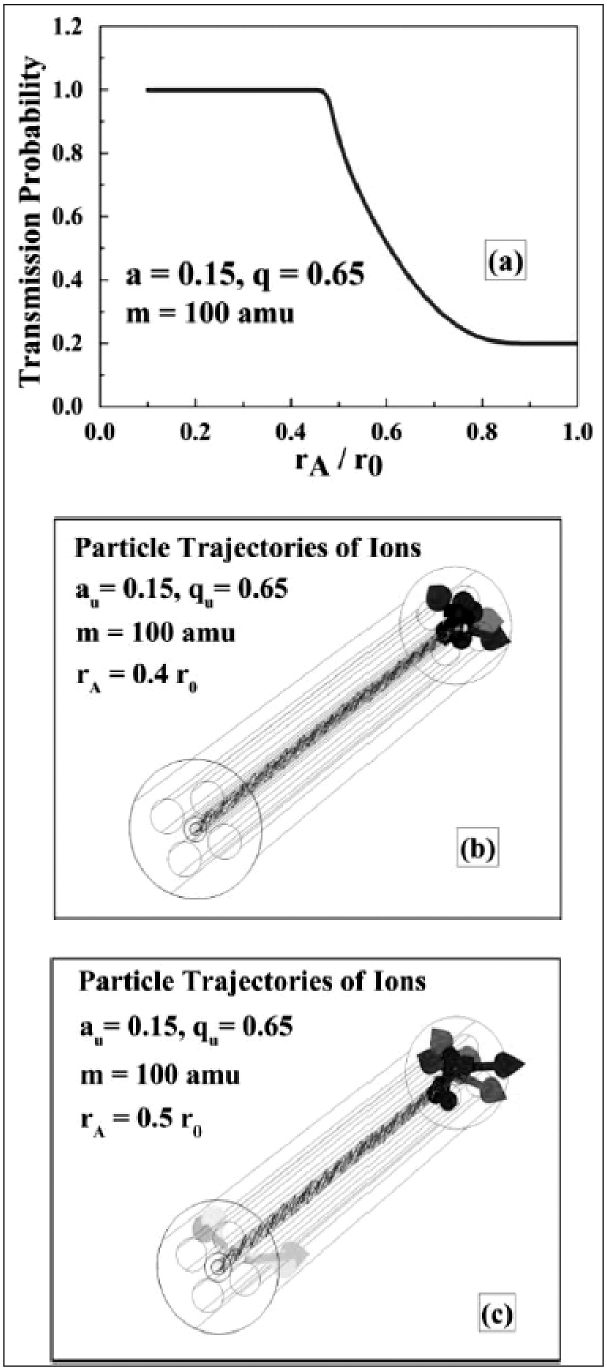

Fig. 7. (a) Transmission probability of ions verses r_A/ r_0 (b) The 2D plot of ion transmission for r_A=0.45 r_0 (c) The 2D plot of ion transmission for r_A=0.5 r_0.

discussed before the use of this focusing voltage 'V_F' will enhance the transmission of ions. At the same time, the magnitude of such voltage should not alter the employed hyperbolic potential for the mass filtering action of ions. It is found from the simulation that the magnitude of V_F has to be less than the DC voltage at the quadrupole electrodes. The 2D plots of hyperbolic potential for the ions of 100amu are presented in figure 5 for different V_F. When V_F > U, the hyperbolic potential of the QMF is perturbed as shown in figure 6.

3.5 Limit on the focusing slit aperture

A circular electrostatic slit with small aperture of radius 70µm is used in the present model to focus the ions into the QMF. The transmission probability of ions for different aperture radius 'r_A' with respect to r_0 is shown in the figure 7(a). When r_A>0.5r_0, the probability of ion transmission decreases gradually. Beside the lower limit of r_A is found to be 0.025r_0 below which the model is not allowing the ions to enter the QMF. Moreover, it is difficult to make slit with such small aperture. The aperture with radius 'r_A' is meant to drive all the sample ions into the quadrupole field of view with an effective area of πr_0^2. This field effective area is just a virtual circle that is tangent to all the four electrodes of QMF. When r_A increases towards r_0, there exist more chances for the ions to get discharged at the nearby electrodes. But, the r_A which is much smaller than r_0 (<0.5 r_0) will direct almost all the ions into the effective field area, resulting in complete ion transmission. The pictorial representation of ion transmission for two different r_A is shown in figure 7(b) and (c). One with, $r_A = 0.4r_0$ = 87.2µm which allows all the ions to transmit the device. While, $r_A=0.5r_0$ =108.5µm has transmitted several ions with the transmission probability of 0.8.

4. Conclusion

The transmission probability of ions in a MEMS QMF is simulated using COMSOL Multiphysics 5.2. The value of Mathieu parameters, a = 0.15 and q = 0.65 is optimized for the better performance of device. The focusing electrostatic slit with small aperture is used to overcome the impact of randomly entering ions at the QMF. The critical limit on such focusing voltage and the slit aperture are determined for the complete transmission of ions. The ions with initial velocity being close to the axial 'z' direction of QMF will enhance their transmission probability. By increasing the device length, the resolution of device is enhanced but the acceptable mass range is found to decrease. This simulation study on MEMS QMF is about to extent in a more realistic way by including the effects of pressure and temperature. The ultimate aim of the authors is to develop MEMS QMFs for space exploration with the availing MEMS fabrication techniques in their laboratory.

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B. Anitha is working as a Junior Research Fellow in the MEMS Development Division, Laboratory for Electro-Optics Systems (LEOS)-ISRO, Department of Space, Bangalore, India. She is pursuing Ph.D in the field of Semiconductor nanostructures in the Gandhigram Rural Institute - Deemed to be University, Dindigul, India. Her research interests are the opto-electronic properties of low dimensional heterostructures and the development of MEMS Devices.

Gogulapati Supriya received her M.Sc. Physics from Vellore Institute of Technology, Vellore in 2007. She worked as an Optical Coatings Engineer in Hind High Vacuum Company, Bangalore. She Joined as scientist at Space Physics Laboratory, Vikram Sarabhai Space Centre (VSSC-ISRO) in year 2008 and had worked in Planetary instrumentation Group till year 2016. Since then, she joined at Laboratory for Electro Optics Systems (LEOS-ISRO) and working in the area of MEMS. Her main areas of interest are Development of Mass Spectrometers and Instrumentation, Fabrication and development of MEMS Devices for space applications.

Dr. Deepak Kumar Sharma received his MS by Research Degree from Indian Institute of Technology, Mandi, India in 2015 and Ph.D Degree from Indian Institute of Technology, Roorkee, India in 2020. Currently he is working as Scientist at Laboratory for Electro Optics Systems (LEOS), Indian Space Research Organization (ISRO). His Research interest includes MEMS Devices, characterization and modelling of semiconductor devices, non-volatile Memory Devices and Device Circuit Interaction.

Jiju John is presently heading the MEMS Development Division of Laboratory for Electro-optics Systems (LEOS), ISRO, Bengaluru. He has M.Sc in Physics from Department of Physics and M. Tech in Optoelectronics and Laser Technology from International School of Photonics, Cochin University of Science and Technology. He is a part of LEOS from the year 2000. His major area of activity is the development of silicon micromachined sensors and actuators. He is leading the teams developing MEMS based Inclination sensors and Instrument for Lunar Seismic Activity studies (ILSA) science payload for India's Chandrayaan mission. He is also coordinating the activities of MEMS development at LEOS that includes realization of RF MEMS, Micro Heat Pipes, Microvalves, gyroscopes and miniature vapour cells. His areas of interest include structure design, fabrication process development, packaging and reliability assurance testing of bulk silicon micromachined devices.

M.S. Giridhar received the B.Sc. degree from the Ruia College, Mumbai University, in 1993, the M.Sc. degree in physics from IIT Madras, in 1995, and the Ph.D degree from the Raman Research Institute, Bengaluru, in 2000. From 2001 to 2003, he held a post-doctoral position at the College of Optical Sciences, The University of Arizona, USA. He joined the MEMS Section, Laboratory for Electro-Optics Systems, Indian Space Research Organisation (ISRO), Bengaluru, in 2003. His research interests are in silicon micromachining, RF MEMS, and RF packaging.

Ashwini Jambhalikar completed M.Sc. in Physics from Indian Institute of Technology, Bombay. She was with Institute for Plasma research, Ahmadabad before joining LEOS in 2005. Since then, she is working in the area of MEMS. Her main areas of interest are in microfluidics and developing MEMS based valves and MEMS based thermal solutions like Micro heat pipes for space applications.