First principles optimization of mass producible microscaled linear quadrupoles for operation in higher stability regions

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In recent years, there has been a desire to scale down linear quadrupoles. The key advantages of this miniaturization are the portability it enables, and the reduction of pump-power needed due to the relaxation on operational pressure. Various attempts at making linear quadrupoles on the micro-scale were met with varying degrees of success [1]-[3]. Producing these devices required some combination of microfabrication and/or precision machining, and tedious downstream assembly. For miniature quadrupole mass filters to be mass-produced cheaply and efficiently, manual assembly should be removed from the process.

A purely microfabricated quadrupole mass filter comprising of a planar design and a rectangular electrode geometry is proposed. Quadrupole resolution is inversely-proportional to the square of the electrode length, thus favoring a planar design since electrodes can be made quite long. Rectangular rods are considered since that is the most amenable geometric shaped for planar microfabrication. This deviation from the conventional round rod geometry calls for optimization and analysis.

Various permutations of the proposed device design were generated in Maxwell-3D and the potential fields were solved (see Figure 1). The field solutions were exported into a MATLAB script that decomposed the field into equivalent multipole terms in a manner similar to [2]. C_2 is the coefficient corresponding to an ideal quadrupole field, while S_4 and C_6 are the first odd and even higher-order component respectively. This expansion is used to examine the magnitudes of the higher-order components as a function of device geometry and is summarized in Figure 2. In simulations that excluded the housing, we found that the coefficients S_4 and C_6 are minimized when the dimensions of the electrode (B or C) is equal to or greater than the dimension of the aperture (A). Choosing an optimized electrode geometry with A = B = C and including the housing, we found that the distances from the electrode surfaces to the surrounding housing (D and E) should be kept equal to minimize S_4, but at the expense of C_6.

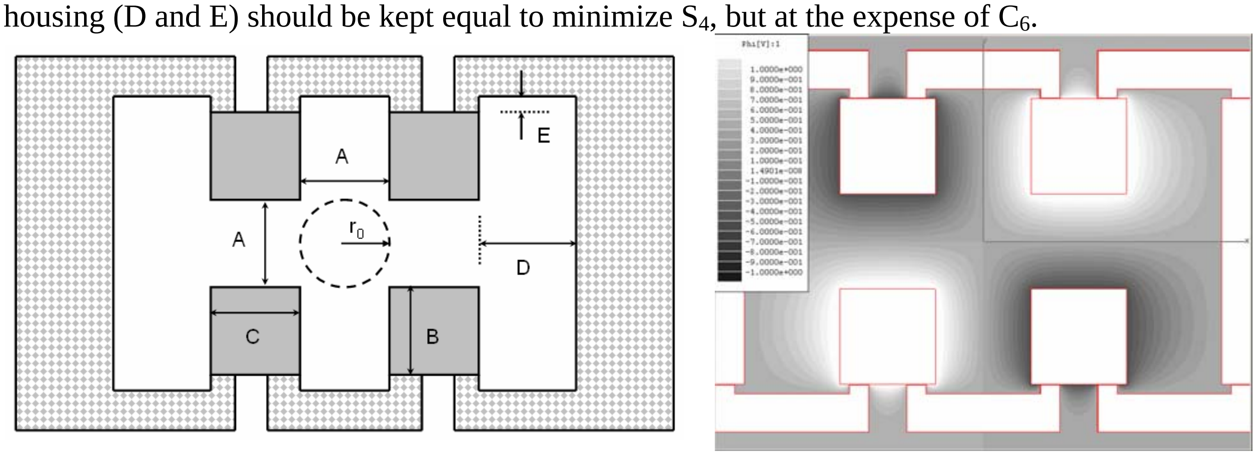

Figure 1 – (*left*) Cross-sectional view of device geometry used in simulations (solid: electrodes, textured: housing). Dimensions A-E are parameterized and r_0 is the effective device aperture radius; (*right*) Maxwell-3D potential field solution for a specified geometry

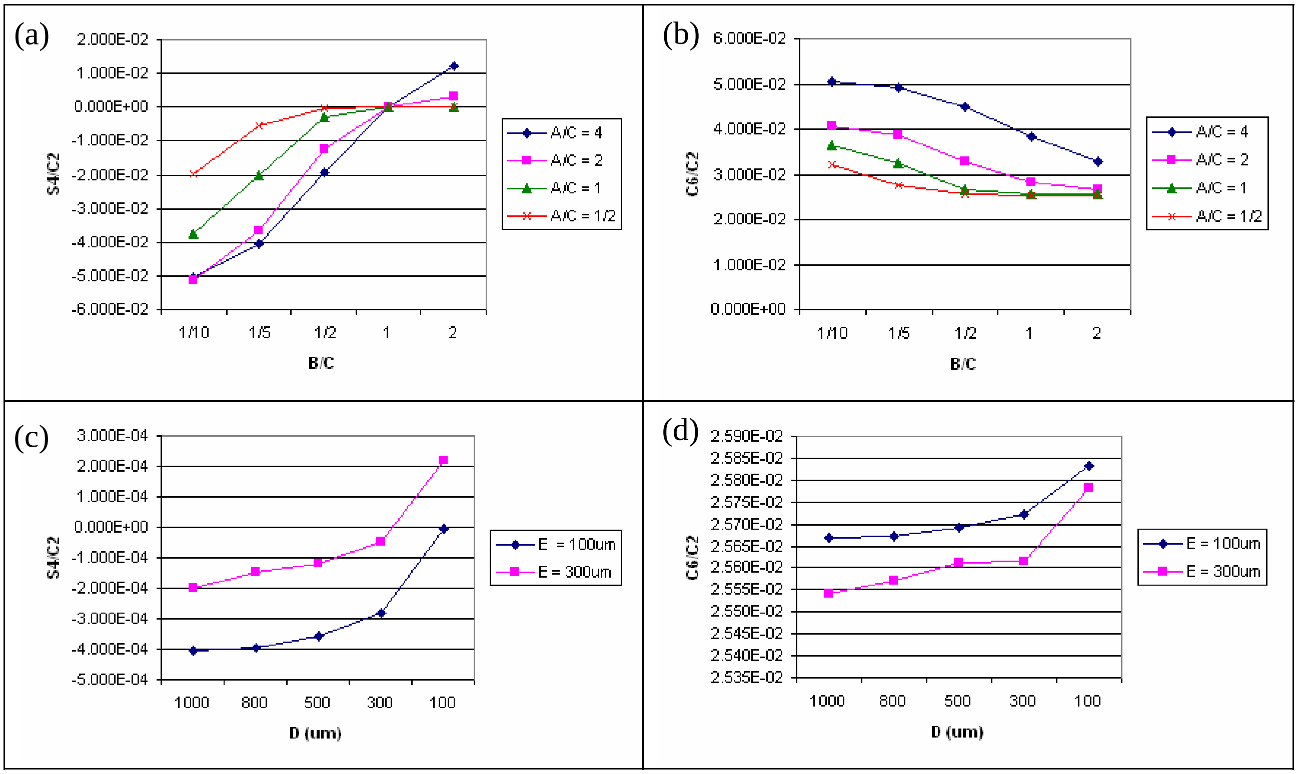

Figure 2 – *Simulation results with electrodes only* (a) First odd higher-order component S_4/C_2 (b) First even higher-order component C_6/C_2; *Simulation results of optimized electrode geometry (A = B = C) with housing* (c) First odd higher-order component S_4/C_2 (d) First even higher-order component C_6/C_2

Higher-order field contributions arising from geometric non-idealities lead to non-linear resonances. These resonances manifest as peak splitting that is typically observed in quadrupole mass spectra. Reported work involving linear quadrupoles operated in the second stability region show improved peak shape without these splits [3]. It is believed that operating the device in the second stability region will provide a means to overcome the non-linear resonances introduced by the square electrode geometry.

We proposed this study to justify the work for a fully microfabricated, mass-producible, MEMS linear quadrupole mass filter. The study indicates that a MEMS quadrupole with square electrodes can function as a mass filter without significant degradation in performance if driven in higher stability regions. Successful implementation of such devices will lead into arrayed configurations for parallel analysis, and aligned quadrupoles operated in tandem for enhanced resolution.

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