COMSOL Based Multiphysics Analysis of Surface Roughness Effects on Capacitance in RF MEMS Varactors

D.Mondal[1], R. Mukherjee[2], D.Mukherjee[1], C.RoyChaudhuri*[1]
[1]Department of Electronics and Telecommunication Engineering, Bengal Engineering and Science University Shibpur, Howrah-711103
[2]School of VLSI Technology, Bengal Engineering and Science University Shibpur, Howrah-711103
*Corresponding author: email: chirosreepram@yahoo.com

Abstract: In this paper, the effects of roughness in the surfaces of the plates caused due to non-uniform etching during their release and/or due to defects in the original wafer on the capacitance in RF MEMS parallel plate varactors are analyzed. Capacitance extraction due to surface roughness has been carried out by mixed mode analysis in three steps: 3D modeling of rough surface in COMSOL, linking of the displacement results with MATLAB for generation of best fit polynomials and evaluation of capacitance by closed form integral expressions. This mixed mode of analysis enables fast computation of capacitances for rough surfaces with different boundary conditions in a flexible manner. The analysis has been carried out on different two plate varactor structures reported by others. It has been found that incorporation of small asperities of 80nm heights in these structures reduces the percentage error in the simulated capacitance from the experimental values by more than 10% which is quite significant.

1. Introduction

MEMS components like switches, varactors and others are being extensively employed in radio frequency circuits to replace bulky off-chip components and also improve the performance of the circuits. MEMS parallel plate varactors improve the phase noise performance of RF VCOs in 1GHz since they have a higher Q-factor than the MOS based capacitors [1]. Various designs of RF MEMS varactors have been reported [2-4] to lower the actuation voltage and improve the tuning range. But, in most of the cases, the measured values are obtained to be significantly higher than the theoretical ones. The discrepancy between theoretical and measured capacitance values can be attributed to (i) parasitic capacitances associated with the capacitor itself or introduced from the bonding/measurement pads, (ii) fringing capacitance, (iii) etching holes, (iv) test set-up configuration, (v) approximation in electrical and mechanical material properties, (vi) residual stress and (vii) surface roughness effects. Amongst these problems, many of them have been addressed. It has been reported that the effect of etching holes is not a major problem and can be accounted during simulation [5-7]. Although the mechanical behavior of the MEMS plate is affected if etching holes are present, the capacitive and electrostatic response remains the same. The mechanical properties of the material like the Young's modulus affect the calculation of the spring constant of the actual devices. The parasitic capacitances in the measurement pads and test setups can be estimated by some calibration methods [8]. The effect of residual stress on the mechanical spring constant of the structures has been reported [9-11] and also the variation of capacitances due to this in parallel plate varactor has been estimated [12]. Impact of surface roughness on the damping factor of MEMS switches [13], dielectric charging effects in pull down capacitance [14] of switches and others have been found to be significant. But the effect of surface roughness on the capacitance of parallel plate MEMS varactors has not been reported earlier.

In the previously reported cases of rough surface analysis, analytical computations were carried out using the different models of rough surfaces like GW model [15] and fractal model [16] to obtain C_{ON} and C_{OFF} primarily. But to analyze the performance of MEMS varactors due to surface roughness, it is essential to compute the capacitances after different deflections. When the plate bends the deflection varies on the surface of the plate and thus the gap between the two plates is different at different locations. To find out the capacitance under such conditions, it is necessary to obtain the displacement of the plate at different locations. An entirely analytical approach has been reported in [17] to compute the displacement and hence the capacitance between flat plate varactors precisely which also requires lesser computational time in the extraction of capacitance than the finite element tool. But an entirely analytical approach for rough surfaces becomes quite complex and also lacks flexibility for adaptation to different boundary conditions. In this paper, we report the effects of surface roughness on the capacitance of MEMS varactors using a mixed mode of analysis. In the mixed mode of analysis, the displacement of a rough surface MEMS varactor is first obtained from the electrostatic module of the finite element tool (COMSOL).The displacement values at different node locations are then imported to MATLAB to obtain the best fit polynomial of the displacement as a function of the spatial coordinates. This polynomial is used to obtain the value of capacitance analytically by closed form integral expressions. The mixed mode of analysis for estimating the surface roughness effects provides the combined advantage of flexibility and less computational time by solving the displacement results by finite element method and the changed capacitance by analytical simulation. The analysis has been carried out for different reported structures of MEMS varactor and compared with experimental results.

2. Mixed mode of analysis of surface roughness effects

In a typical structure of RF MEMS varactor shown in Fig.1, surface roughness can be present either on the two metal plates or on the dielectric surface deposited on the bottom electrode. It is more practical to consider the dielectric slab as the rough surface [14]. The analysis has been carried out in three steps: firstly the 3D model with rough surface has been constructed in 3D builder of COMSOL and analysis is performed to obtain the displacement, secondly the results of the displacement have been imported to MATLAB as a .m file to generate a suitable polynomial and thirdly the extraction of capacitance has been performed analytically by closed form integral expressions.

2.1 Model building and displacement results

The cross sectional view of a typical RF MEMS varactor with a rough dielectric surface is shown in Fig.1.The asperities on the rough surface can be modeled with Gaussian probability density function. Since there is no direct Gaussian function distribution to construct the 3D model in COMSOL, the asperities have been approximated as rectangular blocks of small heights shown in Fig.2. The base areas of the blocks are squares.

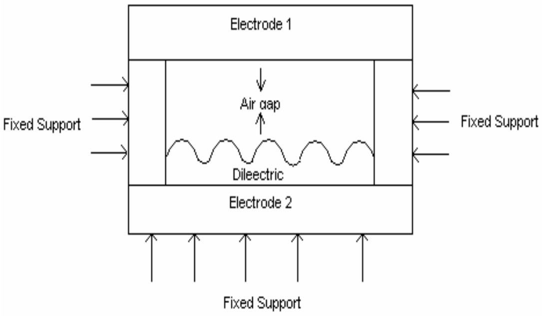

Figure 1. Cross sectional view of RF MEMS with rough surface

This unit has been copied and repeated all over the dielectric surface. Rough surfaces of different asperity heights ranging from 10nm to 100nm have been generated where the thickness of the unit block is 1/10th of the roughness height. The maximum height of the asperity corresponds to the amplitude of the Gaussian probability density function. The width and length of the lowest block have been approximated as six times the square root of variance of the Gaussian function. The cross sectional view of the generated rough surface in COMSOL is shown in Fig.3. The decreasing lateral dimensions of the blocks are the from the Gaussian probability density function at those heights.

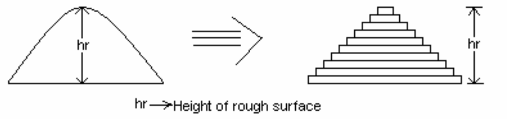

Figure 2. Modeling of a single asperity

Mechanical conditions are applied to the top and bottom electrode of the rough MEMS varactor structure which has been generated using the 3D builder. Next the electrical loads in the form of dc voltages are applied on both the electrodes.

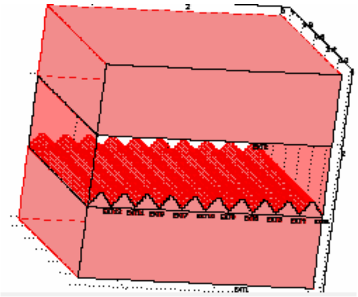

Figure 3. COMSOL model of rough surface

The structure is meshed with finer sizes at the edges of the rectangular blocks and the coupled field analysis is performed to obtain the bending of the upper plate. The capacitance evaluation of this bent structure can then be performed only after reordering the bent geometry and remeshing it once again. This consumes a lot of computational time. To save this, the capacitance analysis of this bent structure is performed analytically. The analysis has been carried out in two parts: generation of a suitable polynomial for displacement to describe the bending behaviour after importing the node results of the bent structure to MATLAB and evaluate capacitance using the displacement polynomial by closed form integral expression taking into account the effect of rough surface.

2.2 Polynomial generation for displacement in MATLAB

The polynomial for displacement has been extracted using the elliptic parabolid, elliptic hyperboloid and general 3rd order polynomial functions. These polynomials have been reported to exhibit greater closeness for fitting a bent electrode due to internal stress [12]. A general elliptic paraboloid, 3rd order polynomial and elliptic hyperbolid expressions are given in equations 1 respectively:

$$z = a_1 x^2 + a_2 y^2$$
$$z = a_1 + a_2 x + a_3 x^2 + a_4 x^3 + a_5 x^2 y + a_6 x y^2 + a_7 y + a_8 y^2 + a_9 y^3$$
$$z = a_1 x^2 - a_2 y^2 + a_3 \tag{1}$$

where, z is the displacement, and a_i represents the i^{th} coefficient of the polynomial or the constants.

The fitting is carried out by Newton Raphson technique since the number of unknown parameters to be fitted is less than the number of experimental values. The fitting of the polynomials is done using MATLAB to generate the values of the coefficient for the least mean square error of 10^{-5}. From the standard deviation of the fitted values using the three polynomials, the one with the lower value is chosen for capacitance extraction.

2.3 Evaluation of capacitance in a rough surface

In a MEMS varactor, the electrodes do not touch each other and the up state capacitance considering a rough surface can be represented in equation 2[18, 19, 20]:

$$C = D_{sum} A_0 \iiint_{x\ -3\sigma_s}^{y\ \ 3\sigma_s} C'(h_r)\,\varphi(h_r)\,dx\,dy\,dh_r \tag{2}$$

where h_r is the height of the asperity tips and it is assumed to have a Gaussian distribution with σ_s as the standard deviation, D_{sum} is the asperity density, A_o is the apparent overlap area, $C'(h_r)$ is the capacitance from one asperity and $\varphi(h_r)$ is the Gaussian probability density function.

$C'(h_r)$ can be expressed as equation 3[20]:

$$C'(h_r) = 2\pi\varepsilon_0 R \ln\left[1 + R/(g_{ma} - h_r)\right] \tag{3}$$

where ε_0 is the dielectric constant of air, R is the assumed constant radius of the spherical asperities, g_{ma} is the gap height between the metal and the asperity mean-height plane which is given by equation 4:

$$g_{ma} = g_0 - z \tag{4}$$

where g_0 is the original distance between the upper and lower electrodes and z is given in equation 1 as the displacement of the upper electrode.

$\varphi(h_r)$ can be expressed as equation 5[20]:

$$\varphi(h_r) = 1/\left(\sqrt{(2\pi)}\sigma_s\right)\exp\left[-0.5(h_r/\sigma_s)^2\right]$$

(5)

Assuming $R/(g_{ma}-h_r) << 1$, $\ln[1+R/(g_{ma}-h_r)] \sim R/(g_{ma}-h_r)$

Thus equation 4 can be simplified as equation 6[20]:

$$C = 1/\left(\sqrt{(2\pi)}\sigma_s\right)2\pi\varepsilon_0 R^2 D_{sum} A_0 \iiint_{x\ -3\sigma_s}^{y\ \sigma_s} \frac{1}{g_0 - z - h_r} \exp\left[-0.5\left({}^{h_r}/_{\sigma_s}\right)^2\right] dx\,dy\,dh_r$$

$$C = \sqrt{2\pi}\varepsilon_0 R^2 D_{sum} A_0 \iint_x^y \left[\frac{2.72}{[g_0 - z]} + 2.66\frac{(\sigma_s)^2}{[g_0 - z]}\right] dx\,dy$$

(6)

Now substituting the suitable expression of ‘z’ from equations 1 in equation 6, we obtain the capacitance of MEMS varactor with rough dielectric surface by equation 7:

$$C = \sqrt{2\pi}\varepsilon_0 R^2 D_{sum} A_0 \iint_x^y \left[\frac{2.72}{g_0} + 2.66\frac{(\sigma_s)^2}{g_0}\right] dx\,dy$$

(7a)

$$C = \sqrt{2\pi}\varepsilon_0 R^2 D_{sum} A_0 \iint_x^y \left[\frac{2.72}{[g_0 - a_1x^2 - a_2y^2]} + 2.66\frac{(\sigma_s)^2}{[g_0 - a_1x^2 - a_2y^2]}\right] dx\,dy$$

(7b)

$$C = \sqrt{2\pi}\varepsilon_0 R^2 D_{sum} A_0 \iint_x^y \left[\frac{2.72}{[g_0 - a_1 - a_2x - a_3x^2 - a_4x^3 - a_5x^2y - a_6xy^2 - a_7y - a_8y^2 - a_9y^3]}\right.$$
$$\left. + 2.66\frac{(\sigma_s)^2}{[g_0 - a_1 - a_2x - a_3x^2 - a_4x^3 - a_5x^2y - a_6xy^2 - a_7y - a_8y^2 - a_9y^3]}\right] dx\,dy$$

(7c)

$$C = \sqrt{2\pi}\varepsilon_0 R^2 D_{sum} A_0 \iint_x^y \left[\frac{2.72}{[g_0 - a_1x^2 + a_2y^2 - a_3]} + 2.66\frac{(\sigma_s)^2}{[g_0 - a_1x^2 + a_2y^2 - a_3]}\right] dx\,dy$$

(7d)

3. Results and Discussions

We have selected some of the MEMS varactor structures reported in [2, 4, 12, 21, 22] where the experimental capacitance curve has been found to deviate significantly from the simulated result. In these structures we have incorporated surface roughness of different asperities on the dielectric and simulated the capacitance values and compared experimentally. The first structure considered is a standard parallel plate capacitor reported in [12] of dimensions 325µm by 325µm with gap between the electrodes as 0.75µm. In absence of applied voltage z is zero in equation 6 and the off state capacitance in presence of surface roughness can be evaluated with the help of equation 7a:

The parameters of the Gaussian probability density function in equations 7 are computed from the following conditions:

$$\text{Max. height of the asperity} = 1/\sqrt{(2\pi)}\sigma_s$$

(8)

$$R \sim 3\sigma_s$$

$$D_{sum} = n\pi R^2/A_0$$

Table1 shows the off statecapacitance values for different asperity heights of roughness. The ideal capacitance of the structure is 1.25pF and the measured off-state capacitance is 2.6pF. It is observed from table 1, that including an asperity height of 80nm makes the simulated capacitance almost 1.86pF which is significantly closer to the experimental value. With further increase in asperity height, the capacitance value increases further. The percentage error decreases by almost 23%. The remaining deviation from the experimental value may be due to the presence of other factors like built-in stress, fringing effects and others.

Table1: Up-State capacitance values for different asperity heights

Asperity Heights(nm)	Simulated Capacitance value(pF)
0	1.25
50	1.35
70	1.54
80	1.86

A two-plate tunable capacitor structure reported in [21] is considered. The structure is suspended with four beams on the sides and the effective area of the plate is 426µm by 426µm with an air gap of 0.75µm. The ideal capacitance in the OFF state is 2pF and the measured capacitance is 4pF. Incorporation of surface roughness of 80nm asperity heights make the OFF state capacitance 2.9pF which is much closer to the experimental value. Electrostatic simulation has also been carried out in this structure. For electrostatic simulation, coupled analysis using finite element COMSOL tool has been carried out. 3D rough surfaces have been created by specifying the function in appropriate coordinates as discussed in Section 2. COMSOL also allows saving its files as m-type which is MATLAB compatible.

To reduce the number of generated nodes and elements and thus reduce the memory requirement and simulation time, only one quarter of the capacitor is modeled and the resulting capacitance is extracted. The capacitance extraction is done using the energy method where the energy density extracted is integrated over the complete geometry [23]. The mesh generated for evaluation of the displacement on application of voltage are finer at places where the distance between the electrodes is small but are coarser at the other end where the distance between the plates is large. The displacement of the electrode generated from COMSOL for an applied voltage of 0.7V with and without surface roughness are mapped into the polynomials and the resulting curves for the polynomials in this structure are plotted in Fig.4. Elliptic hyperboloid has been found to generate oppositely bent electrode geometry and has been not considered. From the standard deviation value computed in MATLAB for both smooth and rough surfaces, elliptic paraboloid polynomial is considered for computation of capacitance. The capacitance vs voltage curve for both smooth and rough surface is plotted in Fig.5 along with the experimental results. It is observed from Fig.5 that incorporation of surface roughness effects make the capacitance value approach the experimental value closely over the entire range of applied voltage. The capacitance value at 0dc bias has been calculated analytically from equation 7a.

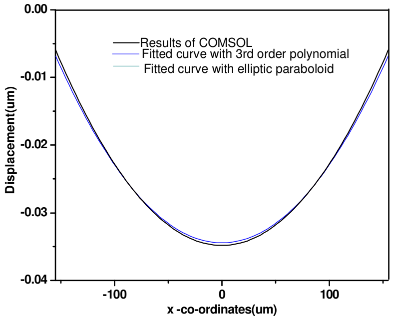

Figure 4a. Displacement curve generated in MATLAB with different polynomials for smooth surface at y=0

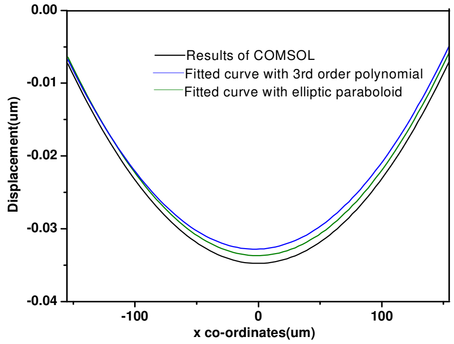

Figure 4b. Displacement curve generated in MATLAB with different polynomials for rough surface with 80nm asperity peak height at y=0

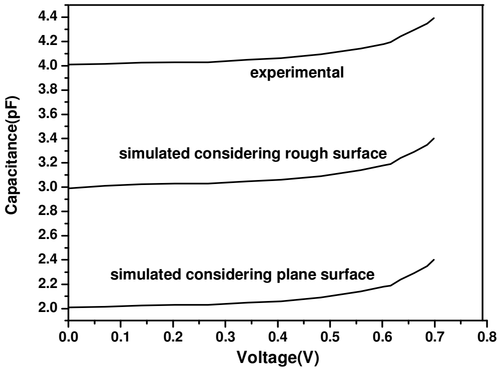

Figure 5. Capacitance vs voltage characteristics

Similar methods have been followed for obtaining the capacitance with rough surfaces for the different structures reported in [2, 4, 22]. In reference [2], the two plate tunable capacitor has effective lateral dimensions of 210μm by 230μm with an air gap of 0.75μm. This structure has been modeled with the four anchors in COMSOL In reference [4], the effective area of the two-plate tunable capacitor is 210μm and 120μm with an initial gap of 0.75μm.There are four anchors to support the structure. In reference [22], the authors used a very thick layer to realize the top plate. The effective lateral dimensions are 250μm by 500μm with a gap of 0.75 μm with the presence of etching holes. For all these structures, surface roughness have been incorporated with Gaussian distribution of asperities with 80nm peak height and the capacitance has been simulated by a mixed mode of analysis and listed in Table 2 in appendix. Elliptic paraboloid polynomial has been obtained to be the most accurate in all of them. The capacitance value has been found to improve in all the cases. However, the remaining discrepancy in the above structures may be primarily attributed to the bending due to internal stress, presence of the fringing capacitance and some of the capacitances that are introduced from the interaction between the signal/ground paths and the movable electrodes.

The deviation is larger in reference [22] compared to the other cases since a very thick layer of 28μm has been used to realize the top plate. In such cases initial deformation due to gravitational acceleration may become significant which might result in an initial increase in the capacitance.

The proposed analysis which is carried out in three steps can be applied successfully for the estimation of surface roughness effects in RF MEMS varactors.

4. Conclusions

In this paper, the effects of roughness in the surfaces of the plates on the capacitance in RF MEMS parallel plate varactors are analyzed. Capacitance extraction due to surface roughness has been carried out by mixed mode analysis in three steps: 3D modeling of rough surface in COMSOL, linking of the displacement results with MATLAB for generation of best fit polynomials and evaluation of capacitance by closed form integral expressions. This mixed mode of analysis enables fast computation of capacitances for rough surfaces with different boundary conditions in a flexible manner. The rough surface has been modeled in COMSOL by constructing hillock like structures on the flat plate of different heights corresponding to different asperities ranging from 10nm to 80nm. The analysis has been carried out on different two plate varactor structures reported by others. It has been found that incorporation of small asperities of 80nm heights in all these structures reduces the percentage error in the simulated capacitance from the experimental values by more than 10% which is quite significant. Thus the methodology proposed in this paper can help in improving the precision of the existing models of MEMS varactors for RF circuit applications without increasing the computational complexity.

5. References

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6. Acknowledgements

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7. Appendix

Table 2: Matching with experimental results

Reference	Measured Capacitance (pF) at 1GHz			Simulated Capacitance(pF) without surface roughness at 1GHz			Simulated Capacitance(pF) with surface roughness at 1GHz		
	0V	2.5V	4.5V	0V	2.5V	4.5V	0V	2.5V	4.5V
2(type 1)	2.05	2.2	3.1	0.6	0.8	1.8	1.2	1.5	2.5
4(type 1)	1.8	1.95	2.5	0.3	0.45	1.0	0.5	0.65	1.25
22	4.6	5	5.1	1.46	1.86	2	2.1	2.41	2.6