Electric Field Assisted Formation of Polymeric Hollow Microstructures


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Abstract:
Hollow microstructures find numerous applications in Microsystems, bioMEMS and microfluidic systems (Unger et al. 2000). Consequently, a one-step fabrication process of hollow polymeric microstructures by external electric field along with capillary forces, termed as electric field- assisted capillarity (EFAC), has attracted the attention of researchers over conventional methods (Chen et al. 2012). Localised higher voltage due to heterogeneous electric field over the thin film makes the polymer grow upward and due to capillary forces it flows encapsulating the inner electrode. This study focuses on understanding various important parameters involved in fabrication of encapsulated hollow polymeric microstructures by EFAC by developing a multiphysics computational model.

Keywords: microfluidics, Hollow microstructures

1. Introduction
The widespread use of hollow microstructures is gaining importance in different areas like bioMEMS and microfluidic systems (Unger et al. 2000). Conventional techniques of manufacturing techniques are chemical etching (which creates a cavity by removing a sacrificial layer) and membrane-assisted microtransfer molding method which uses microchannels from soft lithography (Unger et al. 2000; Thorsen et al. 2002; Xia and Whitesides 1998; Choi et al. 2011). The former is very complex from fabrication point of view and the latter also requires copious processes, thus increasing the fabrication time and expensive machinery also adds to the cost. Therefore, EFAC technique which uses a single step of fabrication process using external electric field and capillary forces is achieving significant attention and is studied in detail to overcome the deficiencies of conventional methods mentioned above.

To demonstrate the EFAC process in a lucid way, Solidworks diagrams have been used as shown in Fig 1(a) to (e)). The top black portion is an electrode and a constant DC Voltage is applied on it. Hence, the spatial heterogenity of the electrostatic field is induced by the patterned top electrode. The polymer liquid (red portion) grows upwards under the protrusion of the top electrode due to the higher voltage and electric field causing a greater force, depleting the liquid under the cavity. When the polymer reaches the top mask capillary force becomes dominant. This causes the polymer to coat the top mask forming a hollow microstructure (Fig 1(e))

Figure 1: Sequence of EFAC from (a) to (e)

2. Modelling approach and Governing Equations
Front view of the process as shown and described in Fig 2 shows that we can focus on the symmetry of the process. Hence, we can model only half electrode for gaining insights into the fabrication parameters.

Figure 2: Symmetry and COMSOL geometry
The following assumptions are used while modeling EFAC:
- A 2D non-axisymmetric model is developed representing infinitely long microchannel.
- The polymer is considered to be Newtonian and the upper fluid is air.
- Incompressible Navier–Stokes equations are introduced to describe the flow.
- Both polymer and air are considered to have a uniform dielectric constant.
- Both the Polymer and air have zero free charge in the bulk material.

Electric field is solved using the Laplace’s equation for the voltage
\[ \nabla \varepsilon \nabla V = 0 \tag{1} \]

The initial driving force on the polymer is the dielectric force at the interface between the two fluids which is calculated by:
\[ F = \rho_f E - \frac{1}{2} \varepsilon_0 \varepsilon_0 E \nabla \varepsilon + \nabla \left( \frac{1}{2} \varepsilon_0 \varepsilon_0 \frac{\partial \varepsilon}{\partial \rho} \right) \tag{2} \]

The foremost term uses \( \rho_f \) which is charge density and causes the electrostatic force. Careful look at the second term shows that it because of variation of dielectric constant. Since both fluids are assumed to have constant value of dielectric constant its value exists only at interface. The last one is the result of changes in the density. While density is constant in the bulk, its value varies at the interface and hence it has a non-zero value at the interphase.

The charge at the interface due to the variation in the dielectric constant, can be calculated as a surface charge density \( \sigma \)
\[ \sigma = (\varepsilon_r - 1) \varepsilon_0 E \cdot \hat{n} \tag{3} \]
\[ \rho_f = (\varepsilon - 1) \varepsilon_0 E \cdot \nabla \Phi \tag{4} \]

To conclude, the final form of equation is
\[ F = (\varepsilon - 1) \varepsilon_0 E \cdot \nabla \Phi + \nabla \left( \frac{1}{2} \varepsilon_0 \varepsilon_0 \frac{\partial \varepsilon}{\partial \rho} \right) \tag{5} \]

3. Use of COMSOL Multiphysics

A 2D transient simulation model is developed for Newtonian polymer film which is assumed to be infinite in the third dimension. Figure 3 shows the details of computational domain along with the applied boundary conditions. Meshing was done using Physics-controlled Fine mesh. The modules used are Electrostatics (es) from AC/DC and Laminar two phase flow phase field from Fluid flow.

![Figure 3: Geometry, boundary conditions and mesh (Dimensions in µm)](image)

In Electrostatics (es) module, Electric field is solved using the Laplace’s equation for the voltage. Laminar two phase flow phase field module solves the incompressible Navier–Stokes equation using phase field method and continuity equation.

\[ \frac{\partial \rho \cdot \vec{v}}{\partial t} + \nabla \cdot (\rho \cdot \vec{v}) \cdot \vec{v} = -\nabla P + \nabla \cdot (\mu \overrightarrow{\nabla \vec{v}}) + \rho \cdot \vec{g} + F_g + F_{st} + F_{ext} + F \tag{6} \]

\[ \nabla \cdot \vec{v} = 0 \tag{7} \]

Phase field method was selected ahead of level set method in Comsol as there is no mass conservation in level set method and the former is stable for evaluating surface tension effects at small scale.

MUMPS solver was used and the body force at the interface was added using Global variables.

4. Results

The polymer near the protrusions of the top heterogeneous electrode feels a higher electric force and hence instabilities arise and the due to the force at the interface as mentioned above, it moves towards the electrode. When the polymer touches the wettable electrode surface, capillary forces dominate and hence it flows along the inside layer of electrode. Hence, it encapsulates the electrode and forms a hollow microstructure. This result is shown as below for
200V, Contact angle between top electrode and polymer = 20°

Figure 4: Evolution of the polymer surface over time at 200V and $\theta_E = 20°$ (Red represents polymer and blue represents air)

4.1 Wettable upper electrode surface

The curved surface of the electrode is having a wetted wall condition which is responsible for capillary flow of polymer.

4.1.1 Variation in Voltage:

Wettable upper electrode surface was taken and simulations were done till 1.5s for a range of voltages while keeping the contact angle between the polymer and the upper electrode material at $\theta_E = 10°$ to study the minimum time required for pattern transfer. The following figures (Fig 5) show meniscus rise profile at different voltages.

Simulation showed that there was a marginal change in the morphology of the polymer film when 50V was applied to it till 1.5s and hence would take a lot of time for pattern transfer (fig. 8). After 100 V pattern transfer started to take place whose unsteady state morphology has been shown in the above images.

4.1.2 Variation in Contact angle with constant Voltage

Now a range of contact angles was taken while keeping voltage constant at 250V. The following figures show the meniscus rise profile at different contact angles.

As indicated by Fig 6, changing the contact angle doesn’t have a significant impact as the difference in the times is in milliseconds. So, it’s alleged that varying the contact angle will not have much effect, while changing the voltage will have an effect.

As we know that the process is divided into two regimes, one where electric force dominates and other where capillary force dominates. These results give us an idea about the timescale required for fabrication of hollow structures. It has the effect on speeding up the overall process as the first stage takes a lot longer than the second stage.

4.2 Variation in Voltage for Nonwettable upper electrode surface

Nonwettable upper electrode surface was taken and simulations were done till 1.5s for a range of voltages while keeping the contact angle between the polymer and the upper electrode material at $\theta_E = 170°$. 

Figure 7: Steady state profile of the polymer with a nonwettable upper electrode

Excerpt from the Proceedings of the 2015 COMSOL Conference in Pune
As shown in the Fig. 7, the hydrophobic electrode surface stops the capillary flow which can be used to get patterned depressions having various microfluidic applications. But as we can see in the last profile that in spite of this, as we increase the voltage, the high electric force pulls the polymer upwards in the space giving a bulge shape which is undesirable. Hence there is an upper limit for Voltage for efficient pattern transfer.

4.3 Spatial gradient in applied DC Voltage

All traditional patterning process work to make a symmetric pattern with no consideration on attaining the mechanical strength at a particular location. The need of giving strength at specific points gives the idea to apply a Specific Voltage gradient. An attempt has been made here for giving strength to the structure but rigorous simulations are still required. Instead of a constant DC voltage, a spatial voltage gradient was applied in the model

\[ V = V_0 + m \cdot x \]

Where,

- \( V_0 \) is the minimum starting voltage at \( x=0 \)
- \( V \) is the abscissa of the bottom electrode
- \( m \) is the voltage gradient applied.

Here, the values of it are as shown below

\[ V_0 = 50 \text{ V} \]

\[ m = 5.71 \times 10^6 \text{ V/m} \]

Figure 8: Effect of spatially varying voltage

As shown in the simulation result, it is observed that the top portion can be given much more strength and can be used in many applications. This result makes this technique to be promising in the coming era.

5. Conclusions

In conclusion, simulation results of COMSOL 2D model for EFAC have been demonstrated. The multiphysics model studied various parameters of the fabrication process such as wall contact angle both for wettable as well as non-wettable top electrode surface and the variation in voltage for each case.

![Figure 9: Effect of wettable contact angle vs voltage](image)

It was observed that changing the contact angle will not have much effect in the dynamics and changing voltage will affect the speed of the first stage of the process, where the electric force is dominant. It has very little effect on the second stage, where the capillary force is dominant.

A spatial varying voltage was also applied for giving mechanical strength to the microchannel. Due to a limited availability of experimental data makes it hard to validate the model. However by comparing with the images of the electron micrograph we can get qualitative idea of the process (H. Chen et al 2012). A complete parametric study needs to be done for all of these parameters to arrive at a more generalized conclusion.
6. References


7. Appendix

Table 1: Properties of polymer (PDMS) in simulation

<table>
<thead>
<tr>
<th>Dielectric Constant</th>
<th>Surface tension</th>
<th>Specific Gravity</th>
<th>Simulation Dynamic viscosity</th>
</tr>
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<tbody>
<tr>
<td>2.72</td>
<td>20 mN/m</td>
<td>1.03</td>
<td>1000 cP</td>
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