DYNAMIC SIMULATION OF INTERFACE SHAPES DURING CHEMICAL VAPOR DEPOSITION

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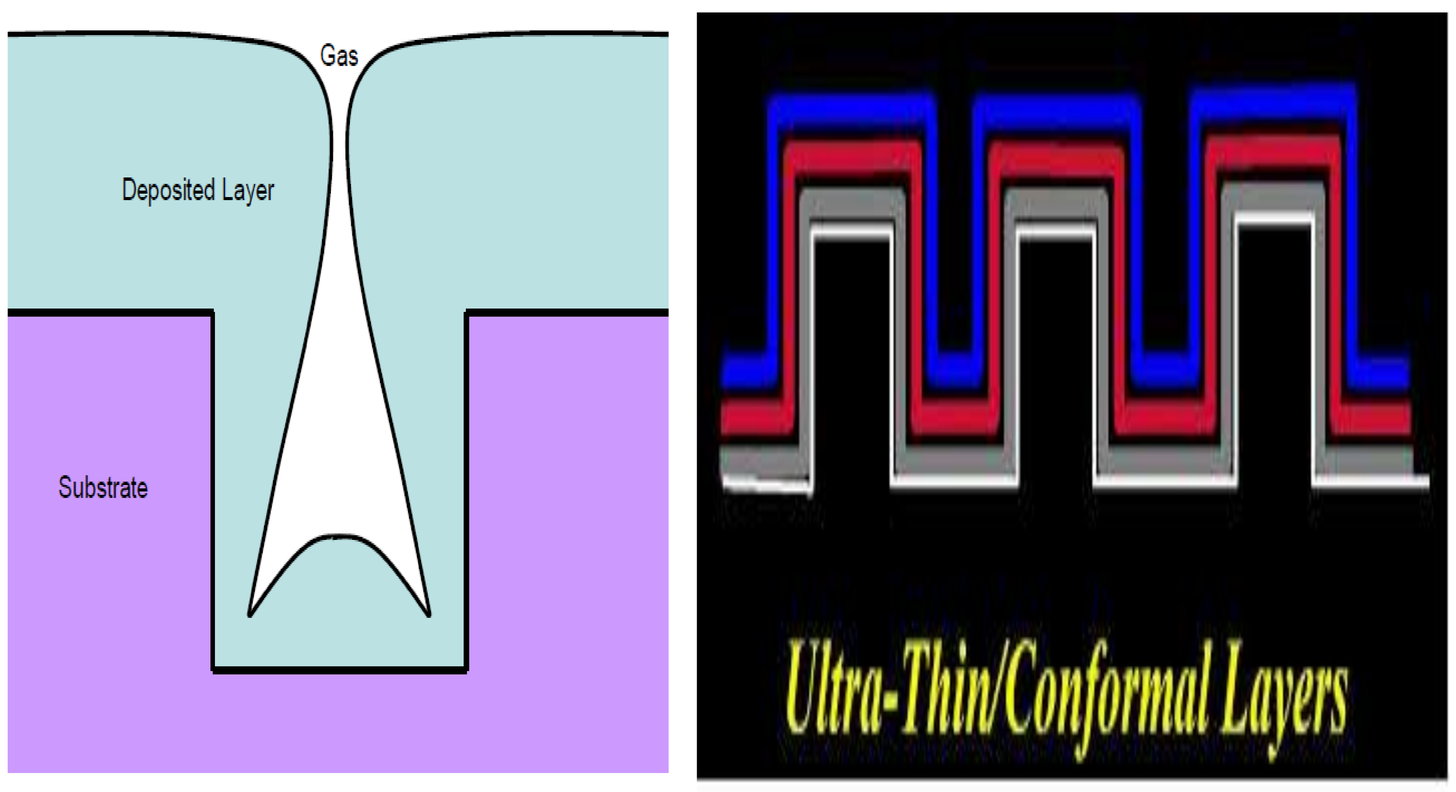
Introduction: CVD finds application in many manufacturing processes of microelectronic devices and MEMS as a recent development. It is also useful for preparation of functionalized surfaces in micro-sensor kind of devices. The phenomena that is studied is deposition of a crystalline material for example Silicon from the gas phase substance such as SiH_4. The material gets deposited on a substrate surface due to chemical reaction. The deposition is carried out in a micron sized well where imaging the pattern of coating is slightly difficult. Hence a simulation is developed which can track the moving boundary or the interface of coated material.



Experimental Observation **Ideal Requirement**

Figure 1. Deposition Pattern

Computational Method: The moving boundary or the interface of coated material is tracked using COMSOL Multiphysics® in combination with MATLAB live link. The following reaction occurs on the surfaces of the trench excluding the top surface

$$SiH_4(A) \rightarrow Si + 2H_2(B)$$

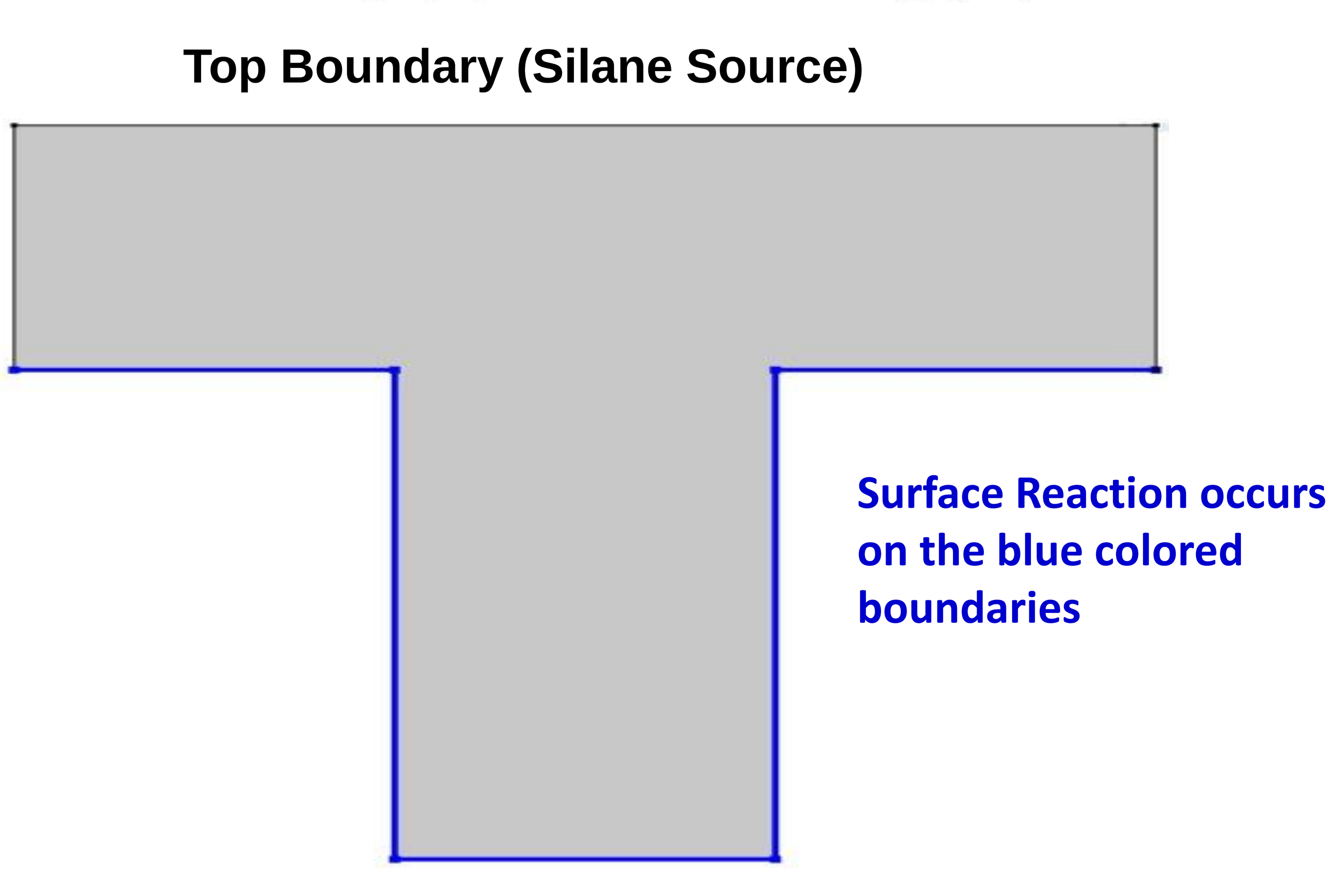


Figure 2. Scaled Geometry of 2D Trench for CVD Simulation

Problem Formulation: Governing Equation and Boundary Conditions for a Process Involving Diffusion and Surface Reaction

$$N_A = Ny_A + J_A$$

$$Where\ J_A = -C_0\, D_{AB}.\nabla y_A,$$

$$N = N_A + N_B$$

$$From\ Stochiometry\ N_B = -2N_A$$

$$So\ N_A = (N_A - 2N_A)y_A - C_0 D_{AB}.\nabla y_A$$

$$N_A = \frac{-C_0\ D_{AB}}{1+y_A}\nabla y_A$$

$$\frac{\partial C_A}{\partial t} = -\nabla.N_A + R_{A,bulk}$$

$$Here\ R_{A,bulk} = 0$$

$$At\ Steady\ State\ \frac{\partial C_A}{\partial t} = 0$$

$$So, \nabla.N_A = 0$$

$$\nabla.\left[\frac{-C_0\ D_{AB}}{1+y_A}\nabla y_A\right] = 0$$

$$At\ the\ top\ boundary$$

$$y_0 = 1$$

$$At\ the\ reacting\ boundaries$$

$$\frac{-1}{1+y_A}\nabla y_A + \frac{k_r}{D_{AB}}\ y_A = 0$$

Results:

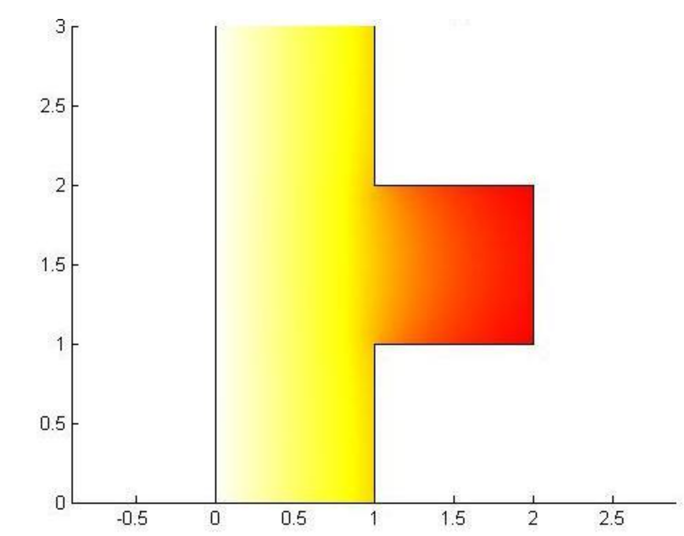


Figure 3. Initial Mole Fraction Color Map at time t=0

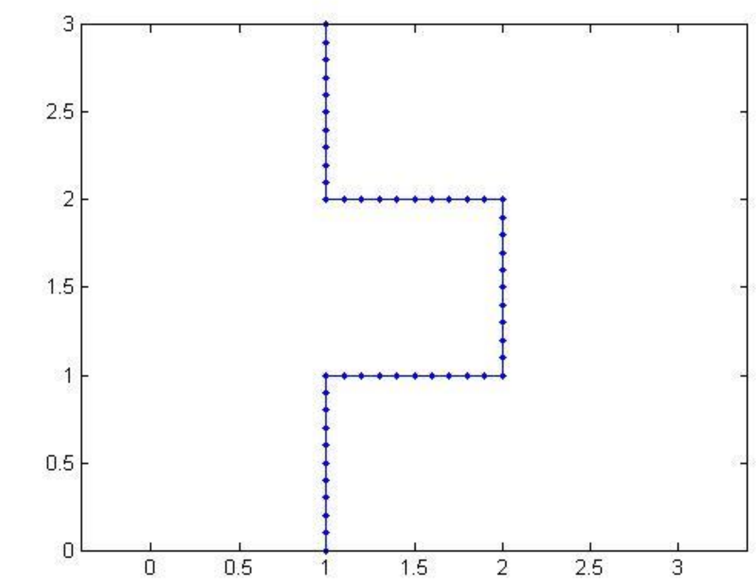


Figure 4. Initial Trench Profile at time t=0

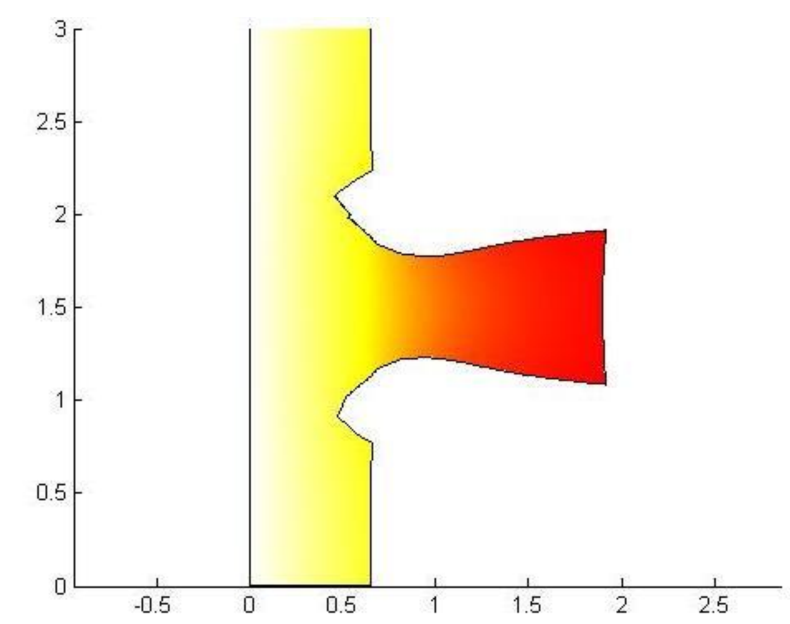


Figure 5. Mole Fraction Color Map at 100th time step

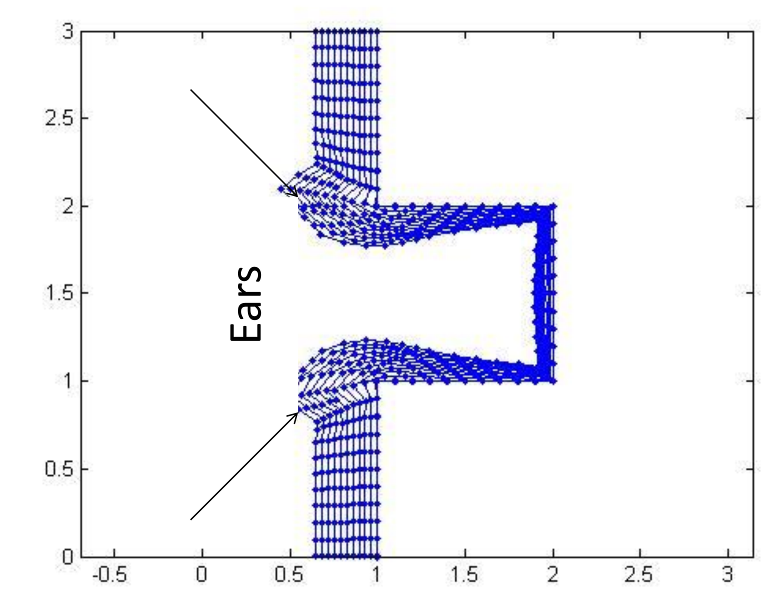


Figure 6. Trench Profile at Various Time Steps

Variable	Value	Units
Temperature	973	K
Pressure	1	atm
Reaction Rate Constant	8.272×10^{-4}	m/s
Diffusivity	2.67×10^{-4}	m^2/s
Depth of the Trench	2	Scaled
Width of the Trench	1	Scaled

Table 1. Simulation Parameters

In the current simulation work the dt = 0.01 units and dx = 0.1 units for the system to have stable interface. It is important to note that the time step and the internodal distance should neither be too small nor be too large for the system to be numerically stable

Conclusions:

1. COMSOL in combination with MATLAB live link can be used to simulate CVD process
2. Our approach of modeling CVD by *Moving Boundary Method* has shown similar geometric shapes of ‘***Ears***’ and ‘***Voids***’ during CVD on a rectangular trench
3. Future scope could be carried out to generate conformal deposition layers by modifying the operating parameters of CVD such as initial geometry and temperature of the chamber

References:

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2. B.Sell et al., Chemical vapor deposition of tungsten silicide (WSi_x)for high aspect ratio applications, *thin solid films*, 443, 97-107(2003)
3. Takashi Nakamura, Novel Pulse Pressure CVD for Void Free STI Trench TEOS Fill, IEEE,117-120(2001)