SIMULATION OF THE ELECTRICAL PROPERTIES OF CONDUCTIVE ITO THIN FILMS BY FINITE ELEMENT ANALYSIS

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Motivation

- Finite element analysis (FEA) can be used to investigate the expected electrical response of materials and devices and compared to experimental results where possible
- Previous work was done on insulating films deposited on conducting substrates (Kumar and Gerhardt, *COMSOL Proc. 2009* and *Meas.Sci.and Tech.*, 2012)
- Effect of film thickness, electrode size, substrate conductivity and film conductivity have also been done (Jin, Kumar and Gerhardt, *COMSOL Proc. 2015*)
- Why study ITO?
  - ITO is the primary transparent conducting material used in the majority of optoelectronic applications
  - Properties of films deposited via sputtering are different from solution processed films
  - Solution processed films can be used to direct write circuit patterns in one step via inkjet printing

Model Set Up and Equations

- Used AC/DC module and set

$$-\nabla \cdot \left((\sigma + \varepsilon_r \varepsilon_0 \frac{\partial}{\partial t}) \nabla \mathrm{V} \right) = 0$$

where σ is the electrical conductivity of the material, ε_r is the relative permittivity of the material and ε_0 is the vacuum permittivity (8.854×10^{-12} F/m)

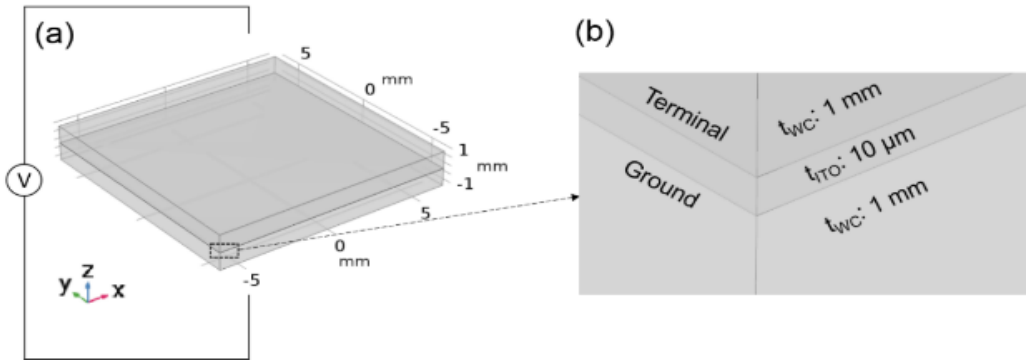
- Materials properties used in the simulation:
  - Air (1.0059, 3 x10^{-15} S/m)
  - Quartz glass (4.2, 1 x10^{-12} S/m)
  - ITO (4*, 1180 S/m)
  - Tungsten Carbide (1*, 5 x 10^{6} S/m)

Modeling Procedure

- Choosing the right 3D model and ac/dc electric currents interface in the COMSOL model wizard
- Drawing films model with or without environment;
- Building the appropriate mesh
- Defining the electrical parameters for each material and boundary
- Computing the model by the right solver in the frequency domain study
- Post-processing the data into other electrical properties

Parallel plate configuration

- Used 2-terminal configurations in 2D and 3D:



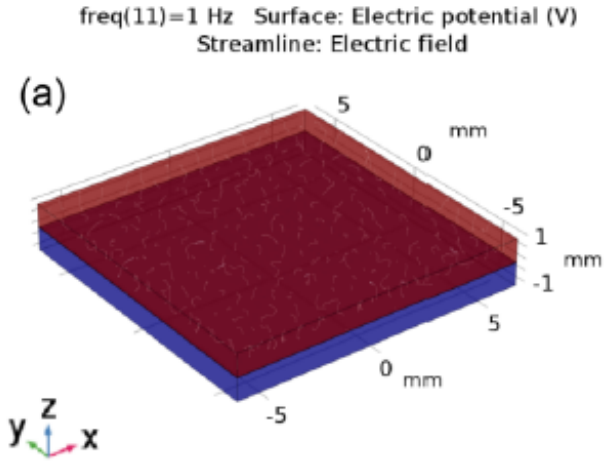
-Top and bottom electrode are

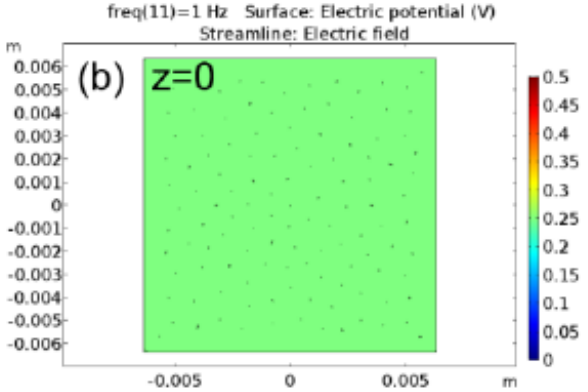
12.7 mm × 12.7 mm x 1 mm thick

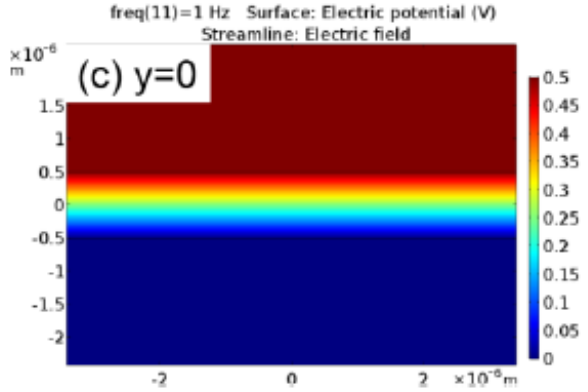
-Film is also

12.7 mm × 12.7 mm but the thickness is 10 μm

Parallel plate results





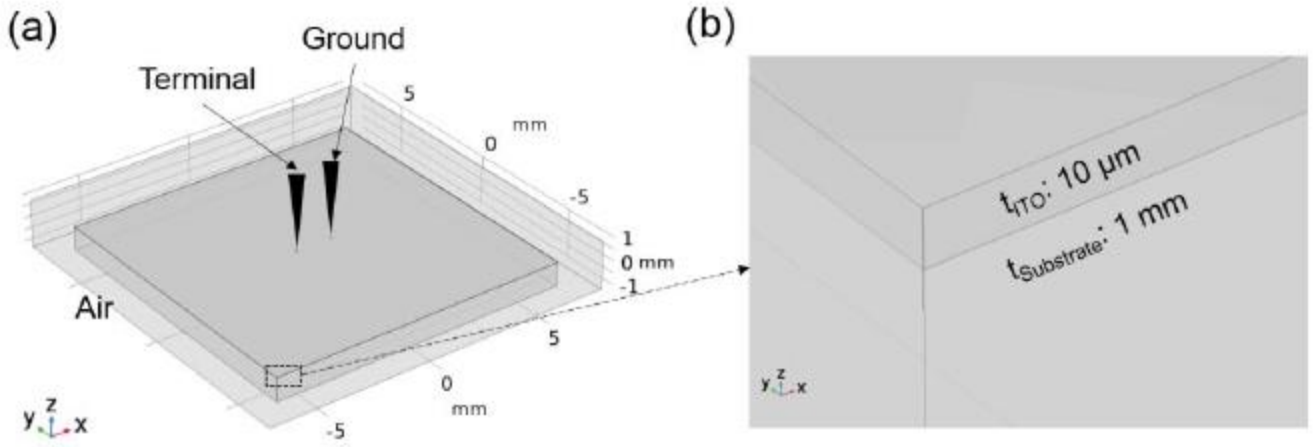


$$\mathrm{R} = \frac{\rho L}{A} = \frac{t}{\sigma a^2} = 5.254 \times 10^{-5}\ \Omega$$

$$\mathrm{C} = \frac{\varepsilon_r \varepsilon_0 A}{d} = \frac{\varepsilon_r \varepsilon_0 a^2}{t} = 5.712 \times 10^{-10}\ F$$

- Simulation results agree with theoretical expectations
- Not possible to measure

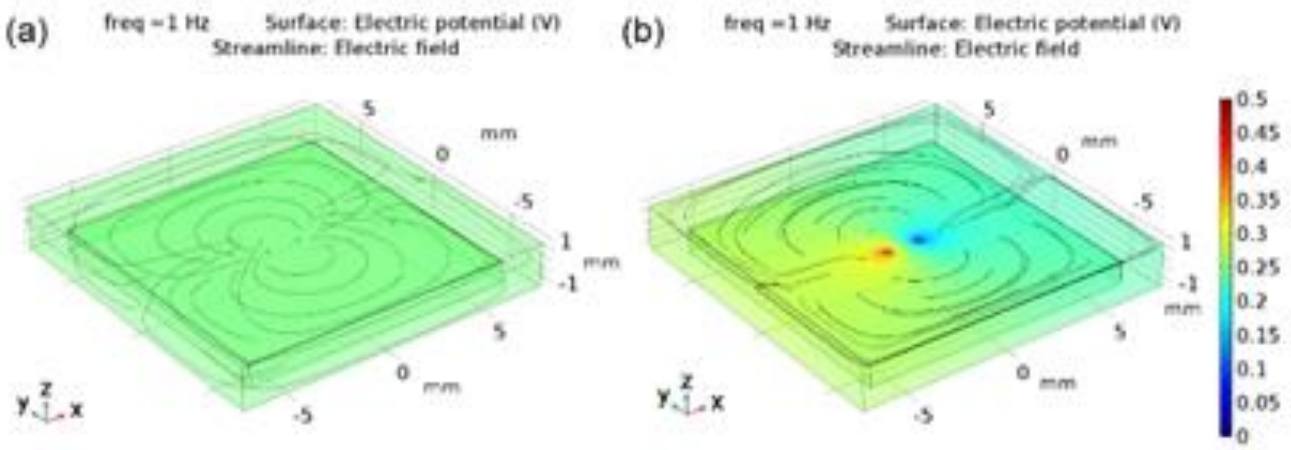
In-plane configuration



(a) 3D model geometry for in-plane measurement configuration
(b) Magnified figure of ITO film on substrate with dimensions

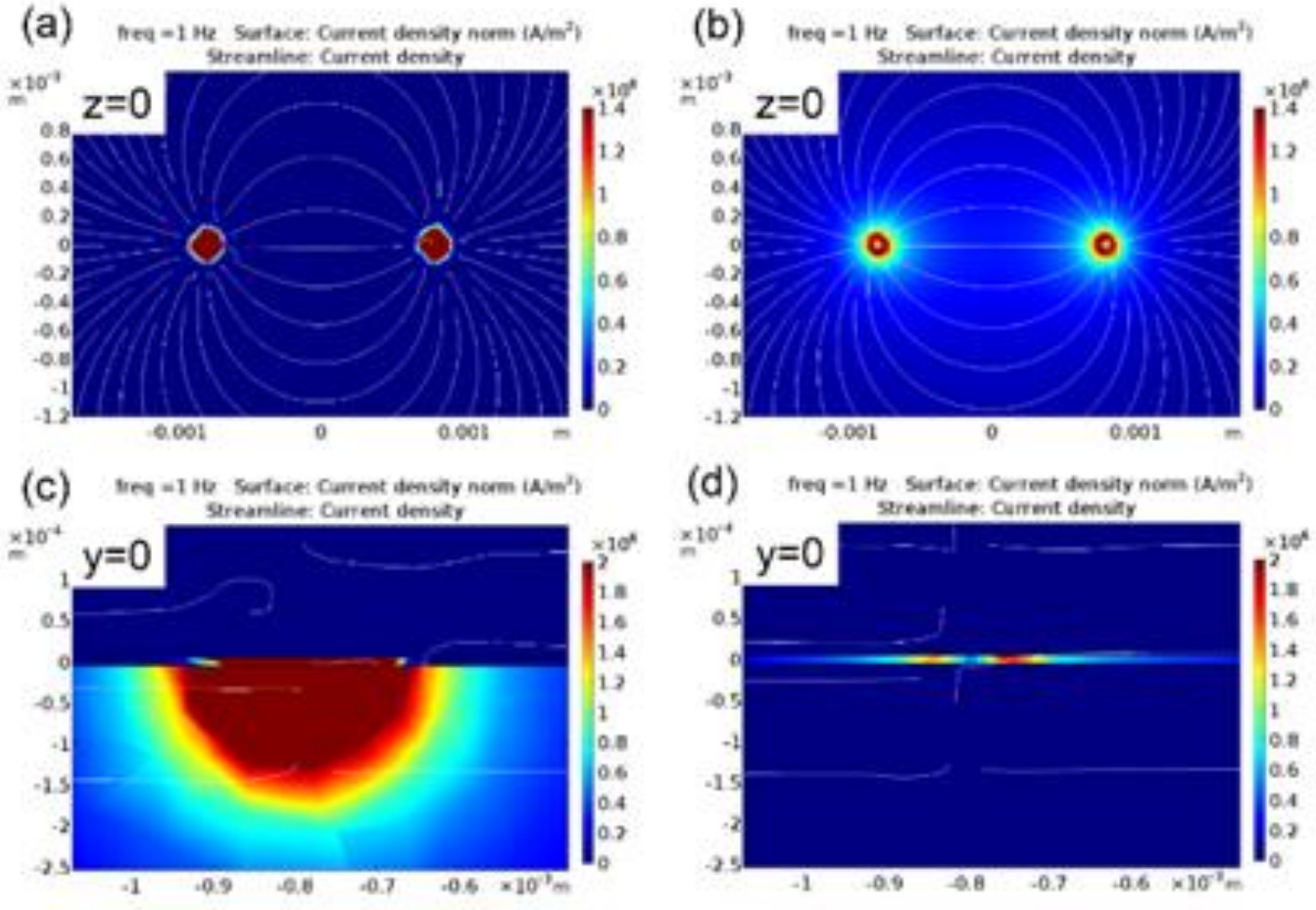
-12.7 mm × 12.7 mm × 10 µm ITO film
-12.7 mm × 12.7 mm × 1 mm substrate,
- D = 80 µm circular electrodes with a center spacing of 1.5875 mm

Simulated 3D Potential maps on conducting and insulating substrates



- (a) ITO film on conducting substrate
- (b) ITO film on insulating substrate

Current density maps on conducting and insulating substrates

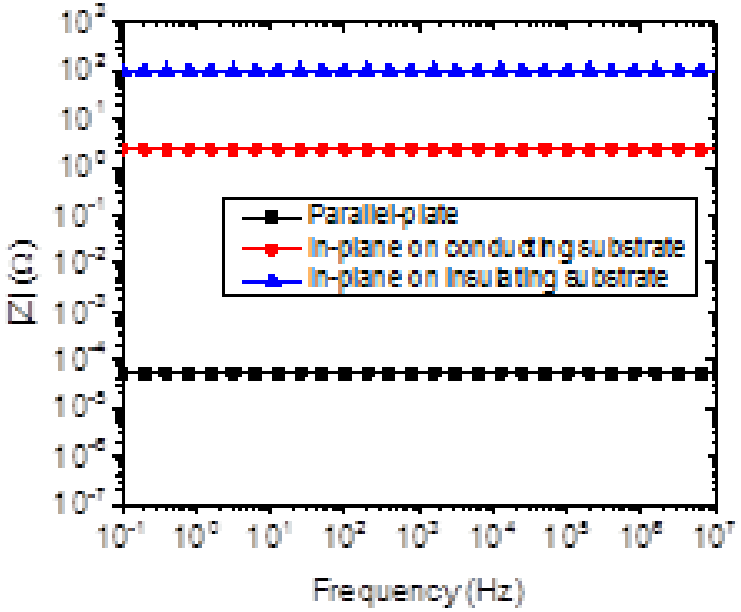


Conducting substrate

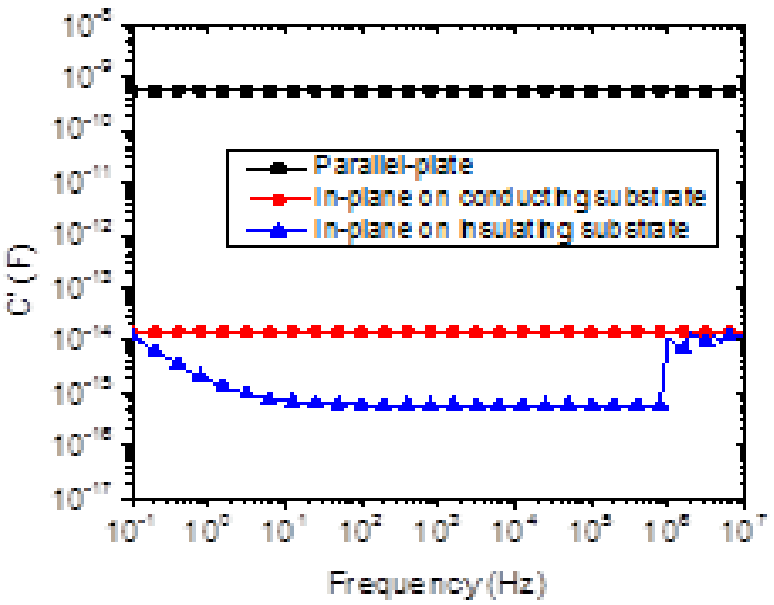
Insulating substrate

Comparison of results with different configurations

(a)



(b)

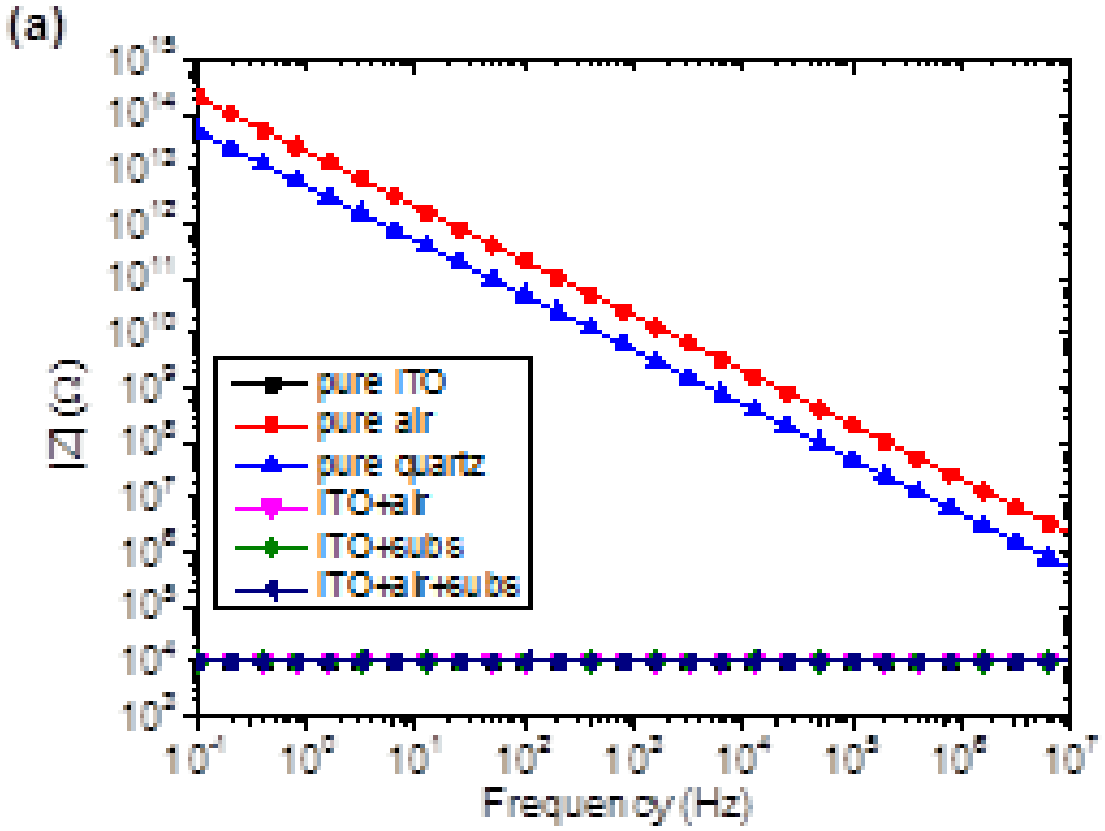


$$Z^* = \frac{1}{Y^*} = Z' + jZ''$$

$$C^* = C' + jC'' = \frac{Y''}{\omega} + j\frac{Y'}{\omega}$$

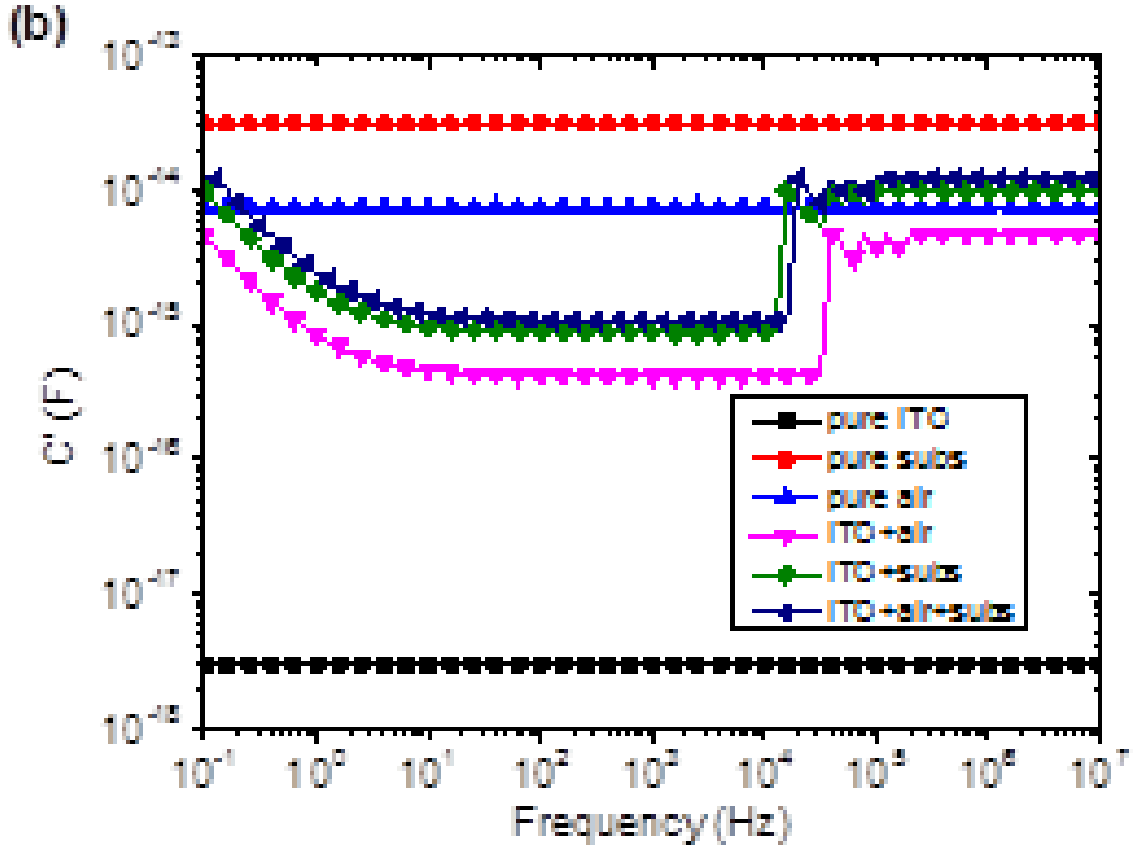
The measurement configuration has a large effect on the resultant properties !! Simulations shown for 10 μm films

Impedance of different combinations



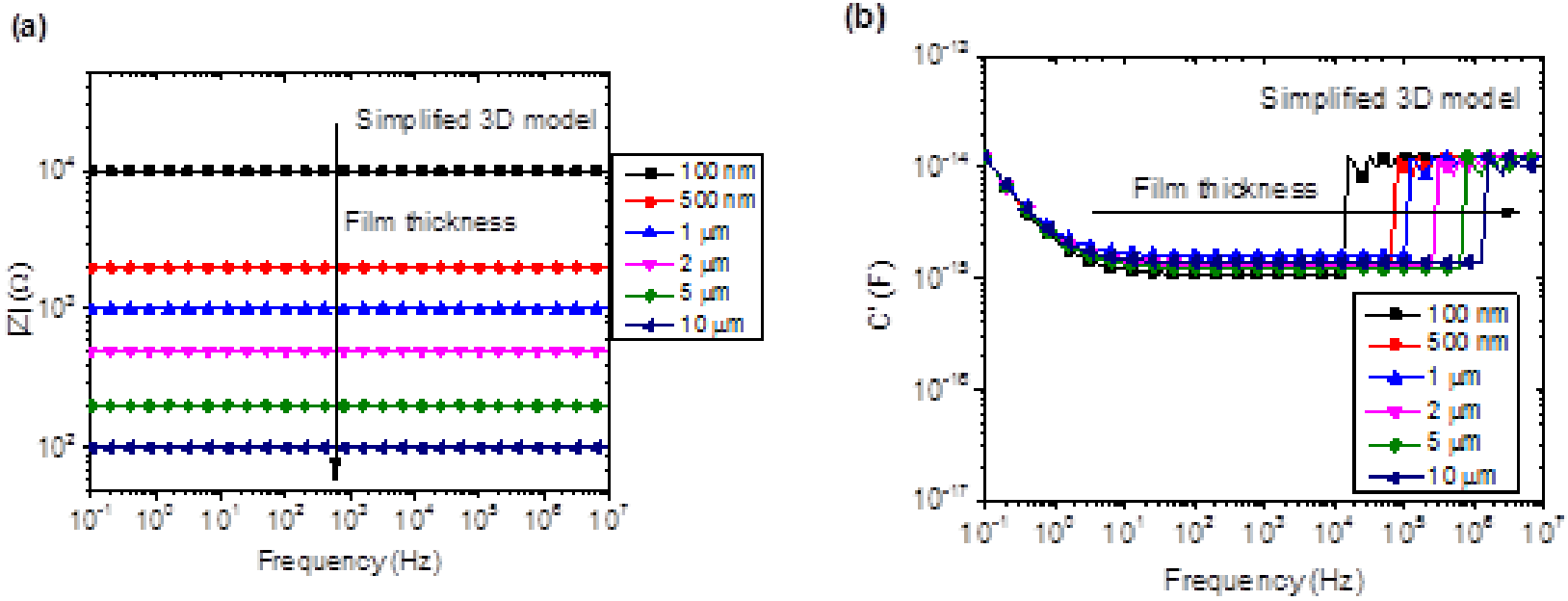
Substrate and surrounding air environment have an insignificant effect on the impedance response of the 100nm ITO films because Z" is very small and therefore |Z*| ~ Z'

Capacitance of different combinations



In-plane capacitance measurement of 100nm ITO film on insulating substrates are dominated by the open circuit capacitance (substrate and air).

Effect of film thickness on in-plane measurements



- Impedance values decrease with increasing film thickness and remain frequency independent
- Capacitance values as a function of thickness are approximately the same below a certain frequency above which the open circuit capacitance dominates

Conclusions

- COMSOL Multiphysics was used to simulate the properties of conducting ITO thin films as a function of
  - Measurement configuration
  - Surrounding environment
  - Film thickness
  - Substrate type (conducting or insulating)
- Results indicate that capacitance response is much more sensitive than impedance to the surrounding environment
- Simulations provided insight for situations where it is currently not possible to obtain experimental data

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