Simulating Ideal and Experimental Impedance Response of Interdigitated Printed Circuit Boards

R. C. Titus[1], R. A. Gerhardt[1], J. E. Fowler[2]
1. School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, USA.
2. Materials Characterization and Performance, Sandia National Laboratory, Alburquerque, NM, USA.

Abstract
Large-scale manufacturing of electronic components require efficient forms of quality testing to ensure bulk fabrication and processing is performed to standard. With numerical simulations, the ideal behavior of such components may be evaluated to better know what to expect. Interdigitated printed circuit boards (PCBs) were simulated to assess ideal impedance responses under varying temperature and relative humidity conditions. The experimental samples compared have copper printed leads on FR4 boards with variation in the application of solder mask, while simulations assumed perfect geometries. The two variations are referred to as coated and uncoated boards. Coated boards have solder mask of roughly the same thickness on the entirety of the PCB, while uncoated boards exhibited multiple regions of varied solder mask thickness in repeating cycles throughout the circuits. This may be due to an error during a negative masking procedure for removing solder mask over the copper combs only. Electrical behavior is derived by utilizing the two-port admittance response gathered after applying two voltage terminals in the Electric Circuits (ec) physics module then converting to impedance. Simulations using copper leads on bare FR4 using the Built-in Material Library are first done due to the exact formulation of the solder mask being unknown. Solder mask properties are then derived by applying a coating of Blank Material over the interdigitated combs and FR4 and setting new material parameters to match that of the experimental results of the coated boards at ambient environmental conditions. To simulate those conditions, Heat and Moisture Multiphysics is performed by utilizing the Heat Transfer in Moist Air (ht) and Moisture Transport in Air (mt) physics modules. A spherical infinite element domain is introduced, where Built-in Material properties for Air is applied to a solid sphere surrounding the PCB. Once ambient properties are normalized for, simulations are performed at varying conditions and compared with experimental impedance responses. The same can then be done for the uncoated boards of greater complexity due to the variations in solder mask thickness. During experiments, topographical characterization using a Keyence 3D Surface Profiler microscope revealed that the solder mask on the circuits held significant levels of porosity, a feature that is further adjusted for in the heat and moisture setups. It is expected for simulations to vary with experimental results due to discrepancies in apparent interdigitated comb heights, large peaks or pores of solder mask, and variation in solder mask application throughout the circuits. The accuracy of final uncoated board simulations with experimental results will boast the usefulness of these methods in making determinations for potential products. With simulations like these, the need for large quantities of demo batches can be reduced significantly.

Keywords: Impedance, dielectrics, permittivity, capacitance, humidity, porosity.

Introduction
Frequency dependency of impedance and dielectric spectroscopy allows for identifying the individual and emergent structure property processing relationships of a sample. Aspects of the response can be discretely isolated by material used, their lumped element parameters, the moisture content adsorbed, etc. [1]. The interdigitated circuit board design is essentially that of a multilayer capacitor, additively increasing in capacitance with every new parallel layer connected. When simulating such samples, parallel RC circuit behavior is found. Unlike that of a pure multilayer capacitor, there is the possibility of current flowing by substrate in addition to the dielectric medium in between electrodes, in this case being solder mask [1]. Finite element analysis methods such as COMSOL allow for evaluations to be done on samples and devices that otherwise are not possible due to the limitations of a research group's laboratory and resources. The objective of this study is to create a model that matches experimental results of interdigitated circuit boards of unknown material composition. Inferences are made using the impedance responses measured in the lab to predict and adjust towards accurate model parameters. The experimental samples were fabricated using copper leads printed on FR4 boards then insulated over the entire circuit using solder mask. Significant levels of porosity was found in the solder mask, increasing the relative humidity (RH) dependency of these samples. Material used to simulate solder mask must allow for moisture dependency of the extracted impedance response. Modifications made to built-in material properties highlight differences between the material composition of experimental samples and ideal samples. Lack of incongruencies in ideal response within simulations highlight defects that may have formed during fabrication or processing of the experimental samples. By analyzing the theoretical and ideal sample predictions, future printed circuit board (PCBs) will rise in accuracy.

Background

General method used with impedance and dielectric spectroscopy equipment is to measure the impedance magnitude $|Z^*|$ and phase angle Θ as a function of frequency [2]. This can then be converted to other impedance functions that help in making sense of the data:

$$Z' = |Z^*| \cos\theta \tag{1}$$
$$Z'' = |Z^*| \sin\theta \tag{2}$$

Where Z' is the real part and Z" is the imaginary part of Z* the complex impedance. Impedance data can be interpreted using lumped element parameters, and the samples examined in this study behave with resistive and capacitive properties. Purely resistive materials exhibit a phase angle of 0 and purely capacitive ones have a phase angle -90 [2]. Dominancy in either property is found along the frequency range, where resistive elements are not frequency dependent and capacitive elements are frequency dependent, decreasing with increasing frequency. In the case of the experimental samples, mainly capacitive properties were found, with slight fluctuations towards resistive behavior at lower frequencies. The format of complex admittance in parallel RC circuit using lumped element parameters is as follows:

$$Y^* = Z_R + Z_C = \frac{1}{R} + j\omega C \tag{3}$$

This is useful for equivalent circuit modeling, where R is the resistor value, C is the capacitor value, and ω is the angular frequency.

Geometry

Interdigitated combs were created using ideal geometries. The rectangular comb dimensions are: 15950 [µm] length, 350 [µm] width, and 50 [µm] height. Gap widths between combs are 250 [µm], 50 combs resulting to 49 gaps. Two main electrodes were used to match that of experimental samples, with 25 combs attached to the main positive lead and 25 to the main negative lead. All combs and leads were set directly on FR4 substrate. The substrate dimensions are: 20950 [µm] length, 31500 [µm] width, and 650 [µm] height. A rectangular slab of height 80 [µm] and same length-width dimensions of substrate was placed directly on the FR4 to act as the solder mask material. This caused an overlap of geometry, solved by using the Difference Boolean between the solder mask and combs to create a specialized geometry that matches the shape of the underlying interdigitated surface. This results in solder mask thickness of 30 [µm] directly above combs. A surface type sphere of radius 31500 [µm] and layer of 10000 [µm] thickness encapsulated the circuit in its center. Air was attributed to the sphere in addition to an Infinite Element Domain of spherical type to better match real world conditions. A fine mesh was created for the circuit, highlighting the FR4 material in blue on Figure 1.

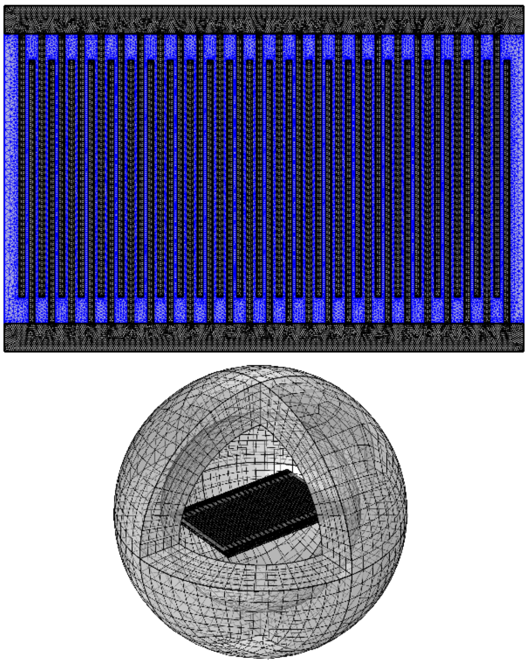

Figure 1. The top image is fine mesh created for circuit, bottom image is mesh for overall system, where transparency is applied to a face of the sphere.

Model Setup and Governing Equations

COMSOL Multiphysics 5.6 was used for this work and ran on an Intel64 Family 6 Model 63 Stepping 2, GenuineIntel using 1 socket with 4 cores. The Electric Currents (ec) physics module within AC/DC Physics was used for impedance response simulations. The Study utilized one step of Frequency Domain, with a range of 10 [MHz] to 100 [mHz] at 15 steps per decade, matching that of the experimental setup. The governing equation is:

$$-\nabla \cdot \left(\left(\sigma + \varepsilon_r \varepsilon_0 \frac{\delta}{\delta_t} \right) \nabla V \right) = 0 \tag{4}$$

where the given electrical conductivity of the material, σ, relative permittivity of the material, ε_r, and the permittivity of vacuum, ε_0, are used to solve for the electric potential [3]. As shown in Figure 2, an electric potential domain terminal is used to apply an AC voltage of 500 [mV] on one side of the interdigitated electrodes, while the remaining half

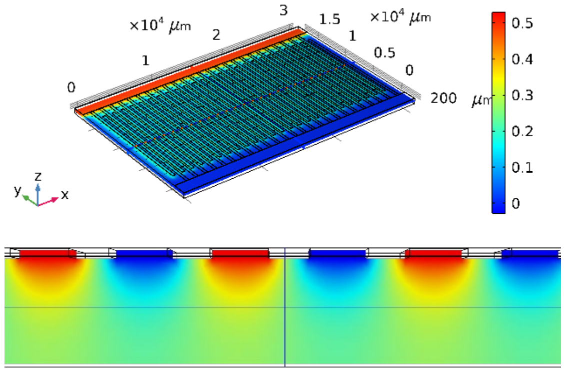

Figure 2. The top image is the 3D Plot of Electric Potential (V) distribution of interdigitated circuits, and bottom is the xz-cross section.

were set with ground boundaries on all surfaces, creating a one-port network seen in figure 2. Once applied, current flowing from the terminal to ground is recorded along with the solved electric potential for each finite element domain, allowing for a calculation to be made for the admittance using:

$$I(\omega)/V(\omega) = Y^* \tag{5}$$

Where I is the current, V is the voltage, and Y* is the complex admittance. COMSOL derives the admittance as a function of frequency, further allowing conversion to the impedance:

$$Z^* = \frac{1}{Y^*} = Z' + jZ" \tag{6}$$

Material properties of porosity can be added and modified, but additional physics modules are needed to implement functions that will make these considerations applicable. Heat and Moisture Multiphysics is used to combine the functions of the Heat Transfer in Moist Air (ht) and Moisture Transport in Air (mt) physics modules. In module (ht), the Porous Medium function was added, which included the subfunctions Fluid and Porous Matrix. In module (mt), the functions Gravity and Moisture Content were added. These added functions were all applied to the solder mask geometry. The Gravity function applied the effects of gravity to the water transport, which would simulate the pooling and sinking of water vapor to droplets on the solder mask surface, and further adsorbing through its porous medium. The rest allowed for identifying the solder mask as the porous medium where interactions will occur, selecting the moisture content on the surface of the mask, and selecting for relative humidity conditions of the surrounding environment.

Discussion

Initially a two-port network was attempted for extracting the admittance response of the circuit. This included a positive voltage domain terminal set to 500 [mV] and a voltage domain terminal set at zero volts as the ground. This resulted in negative real impedance values that may have originated from numerical calculation errors of where current flowed [4]. These inaccurate values were solved by changing the problem to a one-port network described in the Model Setup. With the one-port network, there is only the admittance response directly measuring the response of the sample, allowing for simpler calculations [5]. The calculations also became clear with the inclusion of the combs for the positive voltage terminal and ground boundaries selection. Selection of the main electrodes for the voltage terminal and ground boundaries produced 3D plots that seemed accurate but resulted in confused current density flow. The application of Air through the infinite element domain did not create significant changes to the response of the circuit, however, realistic current density flow was extracted from the 3D plot as shown in Figure 3. This indicates that though a major portion of current flows within the combs, there are various channels by which transport is occurring, via substrate and Air.

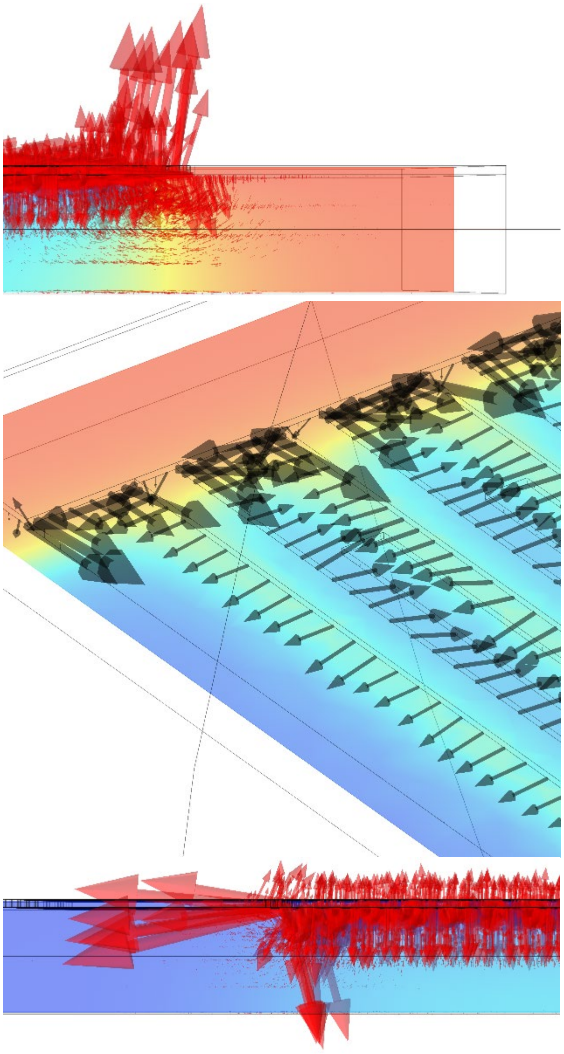

Figure 3. The top and bottom images utilize the Arrow Volume functions to indicate current density flow at the positive and negative main electrodes, respectively. The middle image uses the Arrow Line function to visualize current density flow along and normal to length of interdigitated combs.

Dielectric Properties

Built-in material properties for Copper and FR4 were used to assess the ideal response of interdigitated circuits of this design and property make-up. The properties used are electrical conductivity and relative permittivity. For Copper, the conductivity was $5.998*10^7$ [S/m] and permittivity was 1. For FR4, the conductivity was $4*10^{-3}$ [S/m] and permittivity was 4.5. This results in low frequency real impedance values at the 1kohm range, significantly lower than that of the experimental sample's 5Gigaohms range. Blank Material was then added, overlaying the total surface of the circuit, acting as the solder mask material of unknown composition. Initially, the properties assigned to the solder mask were $1*10^{-7}$ [S/m] and permittivity of 10. This addition resulted in negligible changes in the complex impedance. This is due to current flow being dominated by the more conductive FR4 substrate. The solder mask material must have similar dielectric properties to the FR4 to allow for moisture adsorbed by the solder mask to have a significant effect on the overall impedance response of the circuit. FR4 dielectric properties were then modified to $1*10^{-10}$ [S/m] and relative permittivity of 10, resulting in 10Gigaohms ranged values of real impedance. Comparing the real, imaginary, and phase angle impedance in Figure 4 shows that there is a stark difference between the experimental sample, the unmodified material ideal response, and the modified material ideal response. By dividing the frequency range into three segments, various observations are made. In the low-frequency region, below 10 [Hz], experimental data matches best with the modified ideal, both experiencing similar orders of magnitude in the real impedance, and both transitioning towards more resistive lumped element behavior. The modified ideal's quicker transition to the resistive properties leads to a peak in the imaginary impedance. Following the trend of the

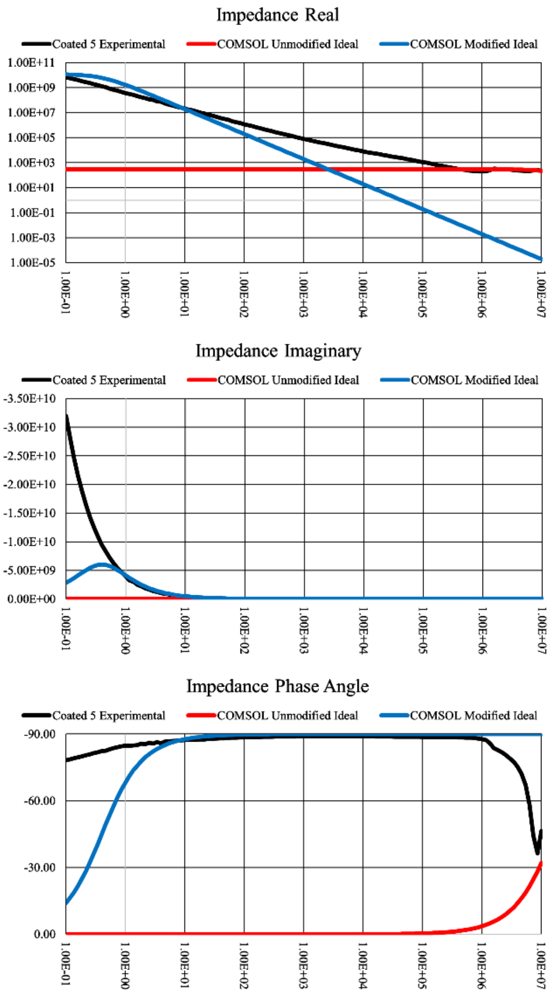

Figure 4. Comparison between experimental impedance response, unmodified ideal material response, and modified ideal material response. The top image is real impedance, middle is imaginary impedance, bottom is phase angle (degrees).

experimental sample towards lower frequency indicates that a resonant peak was nearing formation as well. The experimental sample's resonant peak shift to the left is likely due to additive materials in the material composition that shifts the time constant by influencing the resistive and capacitive elements [2]. In the mid-frequency region, from 10 to 10^5 [Hz], the experimental sample matches best with modified ideal in the phase angle plot, both sharing highly capacitive lumped element behavior. The discontinuity only becomes apparent in the real impedance, where it is found that experimental sample decreases in value at a lower rate than that of the modified ideal. The slope of the experimental sample can be described as between that of the two ideal simulations, with a leaning towards the modified ideal. The obtuse triangle formed in this trio region is the closest opportunity had for all three samples to share an impedance real value, with both simulated responses falling short of the experimental, most extremely at their crossing point. Finally, the high frequency region above 10^5 [Hz] indicate the greatest match with the experimental sample to be the unmodified ideal response. This is most evident in the real impedance where overlap is found between the two. The phase angle then highlights that this is also similar in lumped element behavior, where the experimental sample is experiencing a transition from capacitive to resistive while the unmodified ideal transitions from resistive to capacitive. In the end, the imaginary impedance in this region indicate that all three responses share a value within the same order of magnitude at 10 [MHz]. The unmodified ideal exhibited the least imaginary impedance, and the modified ideal had the most, again indicating a balancing effect that forms a response of similar amplitude to that of the experimental.

Porosity and Moisture Content

Simulations attempting to utilize porous material functionality and surface moisture content both acted upon the solder mask material have not been effective, insignificantly affecting the impedance response discovered.

Conclusions

The high frequency region of the impedance real suggests that the experimental sample's substrate is made of unmodified FR4 to an extent. However, the low frequency region evidently shows that dielectric material does exist in the substrate, becoming dominant at lower frequencies. The experimental samples must be a composite material, with dielectric filler distributed throughout the conductive FR4 matrix. Modifying the geometry of the substrate to include portions that can be assigned dielectric properties will be worked on to bridge the triangular gap in the mid-frequency region.

It is unclear what phenomena creates the smaller slope for the experimental sample found in the real impedance of Figure 3. The slope is uniform in nature, also indicating that there are innate properties of composite material origins. Considering equation (3), the lumped element parameters of passive elements such as the resistor and capacitor do not give rise to clear methods for changing the slope of the imaginary values beyond the trend of increasing or decreasing frequency. Structure effects do not work since changes in the gap width, comb height, etc., would only modify the constant capacitive value in this paradigm.

Progress in creating working model parameters to account for Porosity and Moisture Content is important for making effective predictions about such devices. The effects that were found only created negligible changes in the extracted impedance response. Experimental samples showed significant changes in response due to increases in relative humidity above ambient conditions and most certainly by 65% RH [1]. The experimental cases' greater sensitivity may be attributed to water attaching itself to hydrophilic layers beyond the solder mask and unto the FR4 substrate, further highlighting the importance the material composition for creating accurate models efficiently.

References

[1] R. C. Titus, M. R. Rath, R. A. Gerhardt and J. E. Fowler, "Effects of Solder Mask Variability on the Electrical Response of Commercially Manufactured Interdigitated Circuits," *IEEE Transactions on Device and Materials Reliability,* vol. 24, no. 2, 2024.

[2] R. A. Gerhardt, "Impedance Spectroscopy and Mobility Spectra," in *Encyclopedia of Condensed Matter Physics*, Elsevier Press, 2023. https://doi.org/10.1016/B0-12-369401-9/00685-9.

[3] N. Xia, Y. Jin and R. A. Gerhardt, "Simulation of the Electrical Properties of Conductive ITO Thin Films by Finite Element Analysis," in *2018 COMSOL Conference*, Boston, 2018.

[4] S. Kumar and R. A. Gerhardt, "Numerical Study of the Electrical Properties of Insulating Thin Films Deposited on a Conductive Substrate," in *2009 COMSOL Conference*, Boston, 2009.

[5] M.-C. Tsai and D.-W. Gu, Robust and Optimal Control: A Two-port Framework Approach, London: Springer, 2014.

Acknowledgements

This work was supported in part by the U.S. Department of Energy under Contract DE-NA0003525, and in part by the Georgia Tech Institute for Electronics and Nanotechnology, a member of the National Nanotechnology Coordinated Infrastructure (NNCI), which is supported by the National Science Foundation under Grant ECCS-2025462. The work of Roshaun C. Titus was supported by the U.S. Department of Education GAANN Fellowship. The work of Rosario A. Gerhardt was supported by the Goizueta Foundation Faculty Chair.