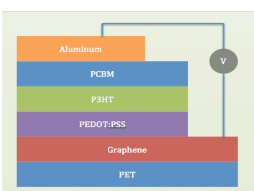
Conductance Modeling of Flexible Organic Thin Film Solar Cell Devices

C. Carradero-Santiago[1], J. Vedrine-Pauleus[2]
1. Materials Science and Engineering, Youngstown State University, Youngstown, OH, USA
2. Department of Physics & Electronics, University of Puerto Rico at Humacao, Humacao, PR, USA

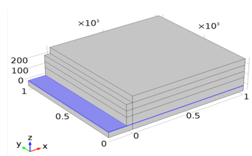
INTRODUCTION: In this research work, we developed a virtual model to examine the electrical conductivity of multilayered thin films when positioned above a single layer and multilayers of graphene, and flexible polyethylene terephthalate (PET) substrate. Additional structured thin films were configure as follows: organic layers of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) as a hole conducting layer, poly(3-hexylthiophene-2,5-diyl) (P3HT), as p-type, phenyl-C61-butyric acid methyl ester (PCBM) as n-type, with aluminum (Al) added as a top conductor. COMSOL Multiphysics was the primary simulation tool used to develop the virtual model and analyze variations in electric potential and conductivity throughout the thin-film structural system. Using the AC/DC Electromagnetic application, electric currents module we defined the geometry of each model and input properties for each tested configurations: PET/graphene/PEDOT:PSS/P3HT/PCBM/aluminum.

We analyzed the model with varying thicknesses of graphene and active layers (P3HT/PCBM). This simulation allowed us to analyze the electrical conductivity, and visualize the model with varying voltage potential, and bias across the plates to better visualize the configurations useful in fabricating organic thin films relevant in solar device applications.



General structure for solar cell device

	Property	Name	Value	Unit
	Coefficient of thermal expansion	alpha	150e−6[1/K]	1/K
	Heat capacity at constant pressure	Cp	1900[J/(kg*K)]	J/(kg·K)
	Relative permittivity	epsilonr	2.3	1
	Density	rho	930[kg/m^3]	kg/m³
	Thermal conductivity	k	0.38[W/(m*K)]	W/(m·K)
	Electrical conductivity	sigma	10e−21	S/m
	Young's modulus	E	1e9[Pa]	Pa
	Poisson's ratio	nu	1	1



Model of Solar Cell on COMSOL

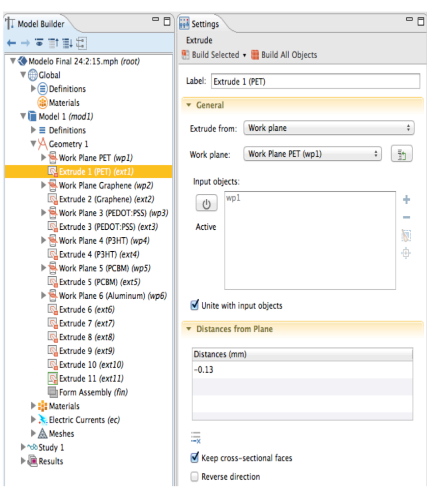


Figure 1. Image of solar cell structure; modeled flexible device; and properties to determine characteristics of materials.

Governing equations used in COMSOL

$$\nabla \cdot \mathrm{J} = Q_J$$

$$\mathrm{J} = \sigma\mathrm{E} + \mathrm{J_e}$$

$$E = -\nabla V$$

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RESULTS:

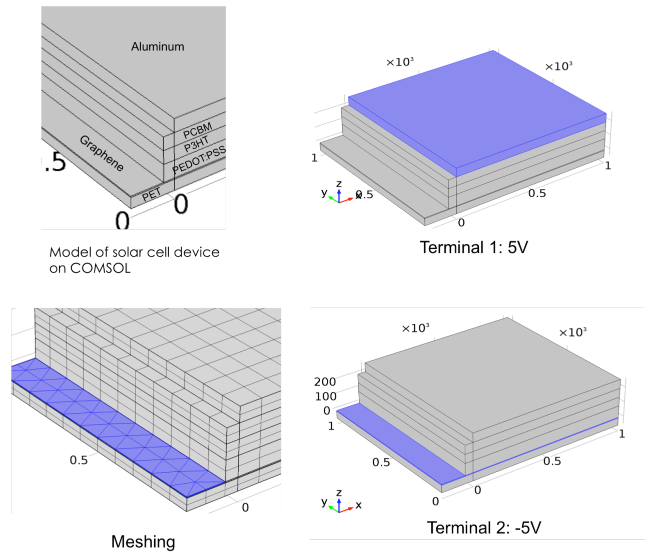

Figure 2. Model configuration, meshing and biasing

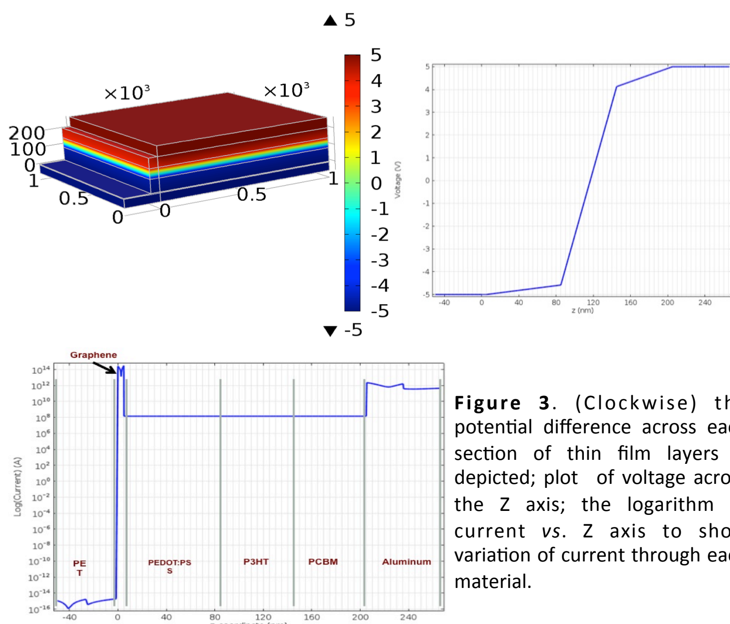

Figure 3. (Clockwise) the potential difference across each section of thin film layers is depicted; plot of voltage across the Z axis; the logarithm of current *vs.* Z axis to show variation of current through each material.

CONCLUSIONS: We analyzed the electrical conductivity across multilayers of thin films to simulate electric potential in a solar cell. We add the electric currents equations and the contact impedance equation to analyze response and behavior of the electric potential across the thin film device. As a result, we obtained a 3D model that shows the behavior of the electric potential across the thin film layers from PET to Al with electrical conductivities of 10-21 and 35.5+6, [S/m], respectively, with a scale bar ranging from dark blue to dark red. The potential between organic polymer layers show variations in colors indicating change in potential with the gradient through the P3HT.

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