Modeling of Nanocomposite Structures to Evaluate the Effect of Nanoplatelet Interphase Region on Electric Field Intensity

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***Abstract*—The effects of the nanoplatelet interphase region on the electric field intensity within a nanocomposite structures are presented in this paper. The modeling of the nanoplatelet and its interphases was performed by using the Finite Element Method Magnetics (FEMM) 4.2 software. Two possible structures of the nanoplatelet were simulated – with and without interphases. In addition, two different models of interphase structures surrounding the nanoplatelet were analyzed – one with rectangular-shaped interphase and the other with circularly-shaped interphase. Both sets of the model interphase were assumed to have different thicknesses and radii. The results showed that the presence of the nanoplatelet interphase affected the electric field intensity of the nanocomposite.**

***Index Terms*—Interphase; Modeling; Nanocomposite; Permittivity.**

I. Introduction

The development of polymer nanocomposites has led the boost of interest in evolving materials for the use in dielectrics and electrical insulation systems [1]. The combination of polymer and a small amount of nanofiller (i.e., polymer nanocomposite) has been found can enhance the thermal, electrical and mechanical properties of the materials compared to its microfiller-added counterpart [1]. The enhancement includes the dielectric properties such as the partial discharge (PD) resistivity, DC breakdown strength, high voltage arcing, and water treeing [2-4].

Polymer nanocomposites nevertheless will exhibit breakdown similar to many pure polymers [3, 5]. Recent researchers claimed that the interphase region, which is a layer between the polymer matrix and the nanofiller is an important region that could contribute not only to unique electrical properties such as increased the breakdown strength, but also it contributes to less favoured dielectric behavior [2, 6-13].

In order to clearly understand the effect of nanoplatelet interphase in nanocomposites, it is important to study the influence of the interphase behavior in nanocomposite materials. Therefore, in this paper, analysis on the effect of nanoplatelet interphase region on the electric field intensity is presented. By varying the structure and the permittivity values of the nanoplatelet's interphase, the results showed that the presence of the interphase can reduce and increase the electric field intensity within the model nanocomposite depends on the structure development.

II. Modeling

A. Parameters

The electrostatic module in FEMM 4.2 was used to model a nanocomposite and analyse its subsequent electric field distribution. A unit cell model comprising a slab polymer with a nanoplatelet was assumed to be placed between two electrodes (high voltage vs. ground) (see Figure 1). The properties of the polymer, the nanoplatelet, and the interphase were assumed as in Table 1. The assumed permittivity values used in the analysis are shown in Table 2.

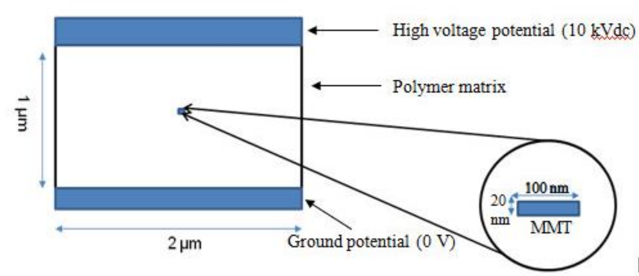


Figure 1: A two dimensional slab with 1 µm thickness and 2 µm width was placed between a 10 kV DC high voltage (HV) electrode and a 0 V ground electrode.

For the ease of simulation, several assumptions were made, such as [6-8]:

- The model contained a nanoplatelet uniform in size,
- The nanoplatelet had interphases which were uniform in size,
- The nanoplatelet were homogeneously dispersed within the polymer,
- The nanoplatelet interacted strongly with the polymer,
- The change in the electric field intensity was mainly affected by the variation in permittivity,

- The change in the electric field intensity was not significantly affected by temperature, and
- The change in electric field intensity was not significantly affected by space charge.

Table 1
Properties for modeling the polymer, the nanoplatelet and the interphase

Material	Size	Permittivity
Polymer	Slab (1 µm x 2 µm)	2.3
Nanoplatelet	Platelet (20 nm x 100 nm)	5.5
Interphase	Depends on the shape of the interphase (see Table 2)	Ranging from 1.5 to 7.5

Table 2
Assumed permittivity values for analysis purposes

Case	Shape of Interphase	Size	Permittivity Polymer	Permittivity Nanoplatelet	Permittivity Interphase
A	None	None	2.3	5.5	2.3
A1	Rectangular	Thickness ,t = 10 nm	2.3	5.5	1.5
A2			2.3	5.5	3.5
A3			2.3	5.5	5.5
A4			2.3	5.5	7.5
C1		Thickness ,t = 40 nm	2.3	5.5	1.5
C2			2.3	5.5	3.5
C3			2.3	5.5	5.5
C4			2.3	5.5	7.5
B1	Circular	Radius,r = 50 nm	2.3	5.5	1.5
B2			2.3	5.5	3.5
B3			2.3	5.5	5.5
B4			2.3	5.5	7.5
D1		Radius,r = 80 nm	2.3	5.5	1.5
D2			2.3	5.5	3.5
D3			2.3	5.5	5.5
D4			2.3	5.5	7.5

B. *Model Description*

As shown in Figure 1, the dimensions of the model nanocomposite were initialized by using a simple polymer slab with thickness of 1 µm and width of 2 µm, placed between a 10 kVdc high voltage (HV) electrode and a 0 V ground electrode. Initially, all models were accomplished by adding a particular permittivity value for the polymer matrix and the nanoplatelet. For simplicity, polyethene with dielectric permittivity, εr = 2.3 was assumed as the polymer matrix while montmorillonite nanoclay (MMT) with εr = 5.5 was assumed as the nanoplatelet. Based on previous findings about nanocomposite interphase models, two possible interphase models were analyzed in this paper. The first interphase model was assumed to follow the shape of the nanoplatelet (i.e., rectangular-shaped interphase with nanometric thickness); this was first introduced by Tanaka et al. [10]. Meanwhile, the second interphase model was assumed to have circularly-shaped interphase; this was introduced by Fabiani et al. [14]. The interphases of the models are shown in Figure 2.

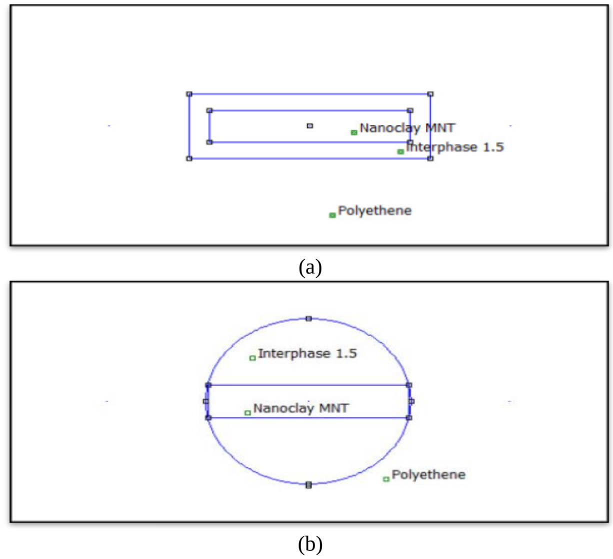


Figure 2: Graphical representation of (a) rectangular-shaped (b) circularly-shaped interphase model.

III. RESULTS

The electric field distribution in an unfilled polymer and a model nanocomposite without interphase is shown in Figure 3. The electric field distribution within the unfilled polymer was homogeneously distributed (see Figure 3(a)), where the electric field intensity was 1.00x106 kV m-1. With the addition of a nanoplatelet within the polymer, the electric field became slightly distorted (see Figure 3(b)). The presence of the nanoplatelet increased the electric field intensity at the region around the nanoplatelet.

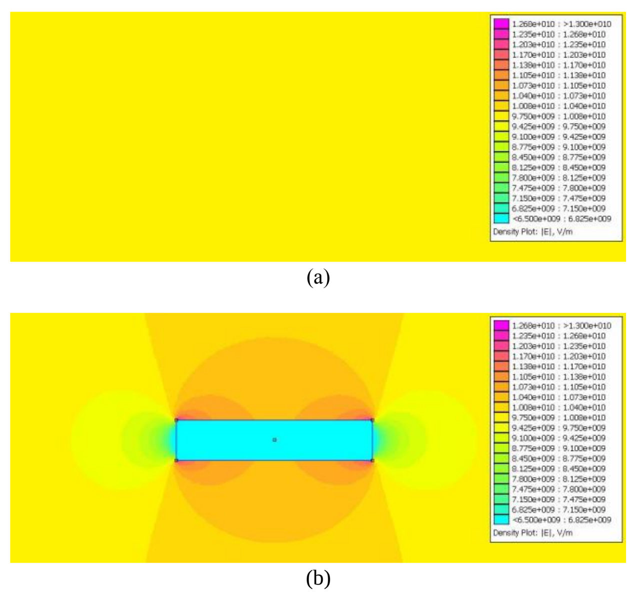
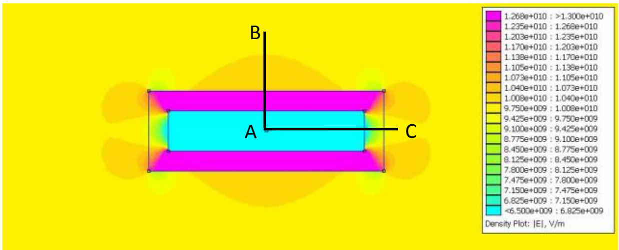
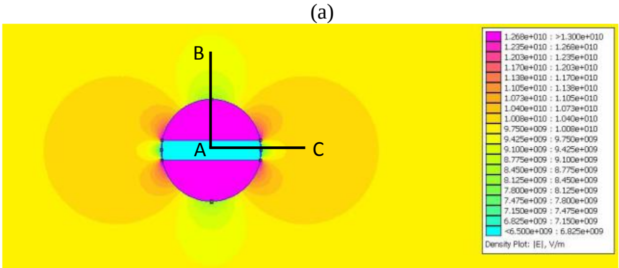


Figure 3: Electric field distribution within (a) a polymer with no filler (b) a nanocomposites in zoom-in illustration

Two different models of the interphase structure surrounding the nanoplatelets were further analyzed, i.e., one with rectangular-shaped interphase and the other with circularly-shaped interphase, as shown in Figure 4(a) and 4(b), respectively. Both sets of the model interphase were assumed to have different values of thickness and radius. The lines AB and AC (see Figure 4) show where the data of electric field intensity were recorded for analysis purposes.



(a)



(b)

Figure 4: Modeling of nanocomposites containing nanoplatelets with (a) rectangular-shaped interphase (b) circularly-shaped interphase.

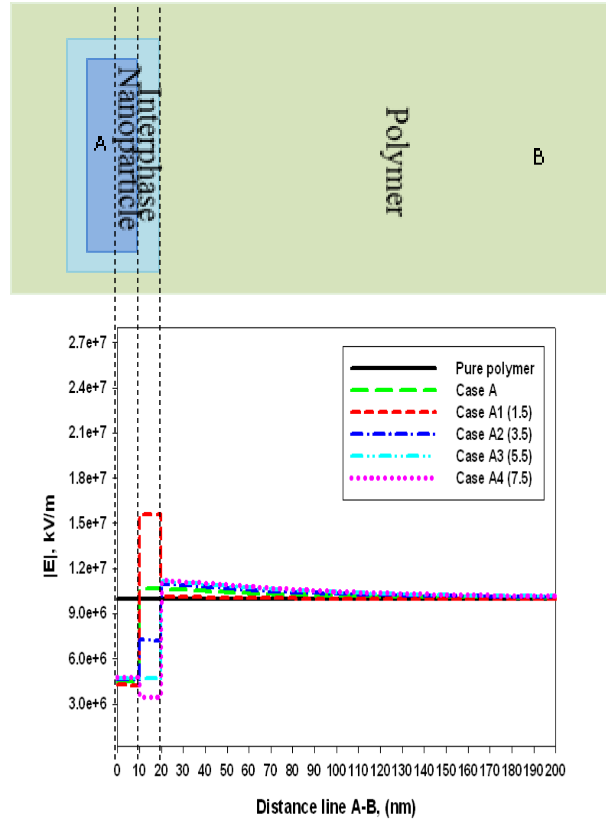
A. Rectangular-shaped interphase model

The analyzed data for the line AB for the rectangular-shaped interphase model was represented in Figure 5. The result showed that the electric field distribution changed within the interphase region when the permittivity values were varied. However, the electric field intensity within the interphase region remained constant.

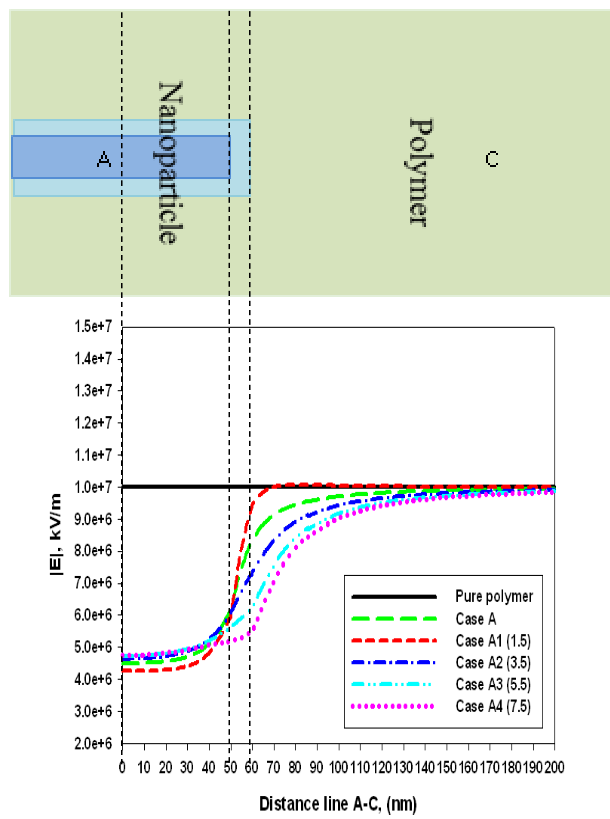
From the analysis shown in Figure 5(a), the electric field intensity within the interphase region was not affected when the interphase permittivity value was set at 2.3 (same as the polymer permittivity value), denoted as case A. At lower interphase permittivity value, which was 1.5, denoted as case A1, the result showed that the value of the electric field intensity within nanoparticles (~4.3x106 kV m^{-1}) was lower compared to case A. However, when considering case A1 within the interphase region, the results showed drastic changes in the electric field intensity; it was much higher compared to other cases (~1.55x107 kV m^{-1}).

Furthermore, for case A3, the permittivity of the nanoparticle was chosen to be similar as the interphase region, which was set at 5.5. The electric field distribution was found to be constant in this region (same value as in the nanoplatelet). At a higher interphase permittivity value, i.e., 7.5, the nanoparticle (referring to case A4) produced the opposite effects to that of case A1.

Figure 5(b) shows the plot of the electric field intensity for line AC. For case A1, the electric field distortion within the interphase region was also at the highest value, which was similar with the analysis for the line AB. Similarly, case A4 gave opposite results from case A1 where, lower electric field intensity was achieved within the interphase region. In addition, as observed from the analysis, the electric field intensity within the interphase became more noticeable.



(a)



(b)

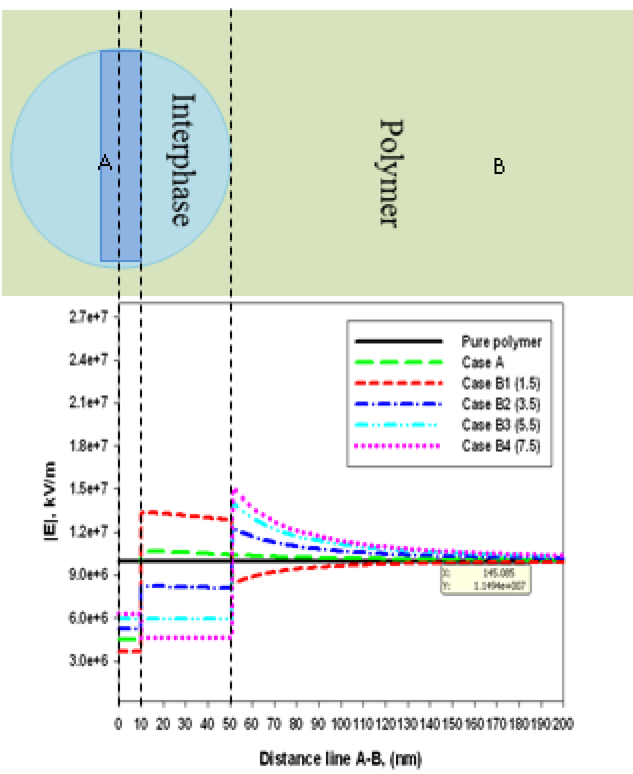
Figure 5: Analysis on the effect of nanocomposites containing one-dimensional (1-D) nanoparticles and the interphase region for rectangular-shaped interphase from the origin. (a) line AB (b) line AC

B. Rectangular-shaped interphase model

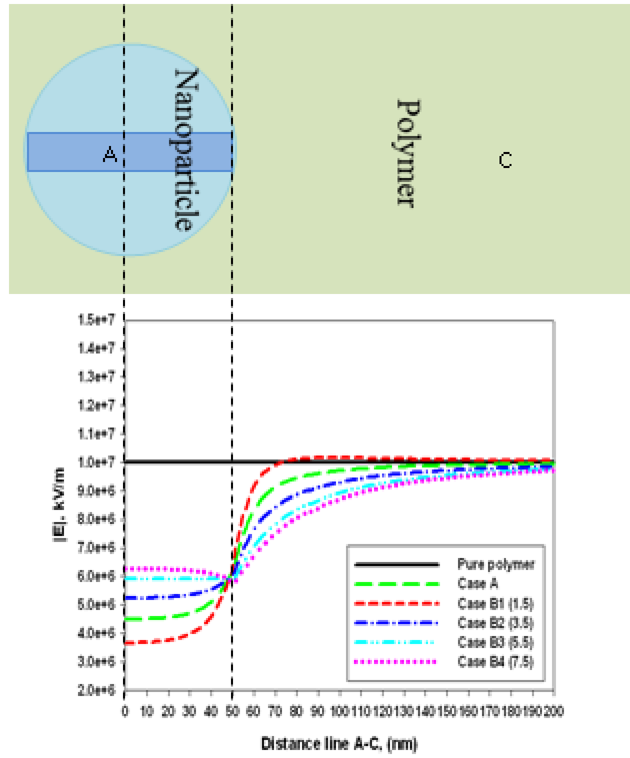
Figures 6(a) and 6(b) depict the electric field intensity plot for the circularly-shaped interphase model. The pattern obtained was different compared to the rectangular-shape interphase model shown in Figure 5(a). The electric field intensity within the interphase region was found to change continuously with a decreasing pattern. In addition, the results show that electric field intensity became higher at the boundary of the interphase and the polymer region.

Besides, based on the analysis for the line AB as shown in Figure 6(a), different patterns of the electric field intensity can be observed at the boundary of the interphase region and the polymer matrix. All of the cases experienced dramatic changes especially for case B4, in which, as the value of the interphase was higher than the nanoparticle (permittivity value of 5.5) and the polymer (permittivity value of 2.3), the electric field intensity at this boundary would increase up to ~1.5x107 kV m^{-1}. However, in this case, the electric field intensity within the interphase region of the circularly-shaped interphase model (~4.7x106 kV m^{-1}) was higher compared to the rectangular-shaped interphase model (~3.4x106 kV m^{-1}). In the case of the interphase region having similar permittivity of the nanoparticle, there was no effect to the electric field distribution found in the interphase region.

When the value of the interphase permittivity was at 3.5, which was between the polymer matrix and the nanoparticle permittivity value (case B2), the result showed that the electric field intensity within the interphase would increase as compared with the intensity within the nanoparticle.



(a)



(b)

Figure 6: Analysis on the effect of nanocomposites containing one-dimensional (1-D) nanoparticles and the interphase region for circularly-shaped interphase from the origin. (a) line AB (b) line AC

However, the value was lower than the electric field intensity of unfilled polymer. Meanwhile, for a higher interphase permittivity value (case B4), which was higher than polymer (permittivity value of 2.3) and nanoparticle (permittivity value of 5.5), the results created opposite effect to the lower interphase permittivity value (case B1). However, the electric field intensity within the interphase region for case B1 significantly reduced compared to the rectangular-shaped model (from ~1.6x107 kV m^{-1} to ~1.3x107 kV m^{-1}).

From the analysis on data for line AC that was depicted in Figure 6(b), it can be summarized that the level of electric field intensity within the polymer was similar with the rectangular-shaped interphase model. Both model having the same pattern as observation on the plot pattern of electric field intensity as observed in Figure 5(b) and Figure 6(b).

However, the electric field intensity within the nanoplatelet became greatly distorted as the values of the interphase permittivity for the circularly-shape interphase model were varied. The electric field intensity within the nanoplatelet became higher (~6.2x106 kV m^{-1}) for case B4 compared to other cases. Lower permittivity values of interphase (case B1) will result in opposite effects to case B4 where lower electric field within the nanoparticle (~3.6x106 kV m^{-1}) will be obtained. For both models, it was observed that the electric field intensity continuously increased up to one constant value (~1.00x106 kV m^{-1}), approaching the permittivity of the unfilled polymer.

IV. Discussion

The drastic changes of the electric field intensity at the boundaries of one component with another component (e.g. from nanoplatelet to interphase regions or interphase to polymer regions) with different permittivity values have been observed in the results section. The changes are due to the forces of the chemical bond occurred between each component. Meanwhile, the forces occurred due to the charge differences between two categories of components. Besides, the formation of the electric layers could generate the electrostatic force between these components and this could contribute to the electro-chemical potential. The phenomenon is known as triboelectricity [10, 15, 16].

Triboelectricity series illustrate that the materials tend to transfer electron between two materials with different polarity. Even though there were no data available for montmorillonite as nanofiller, it could be assumed that montmorillonite was positively charged, while polyethylene was negatively charged because of the drastic change of electric field at the boundary between these two materials. When the process of transferring the electron between these two materials took place, a charge distribution layer forming at the boundary known as Gouy-Chapman diffuse layer could occur [10, 15].

The presence of the interphase region has been claimed as one of the significant roles that can affect the dielectric properties, but the exact value of permittivity for the interphase region is still unknown [8]. In this paper, the interphase region was assigned random permittivity values in order to investigate their effects on the resulting electric field distribution within a nanocomposite system. The electric field was distorted as various permittivity values of the interphase were assigned.

The electrical breakdown depends on the electric field distribution. Therefore, the breakdown that occured due to high field region [7, 17] may correlate with the variations of electric field intensity observed in nanocomposites. The presence of the interphase region depends on the polymer structure and chemical bonding between polymer and nanoparticle [6, 8, 10-12] Thus, the structure of the interphase region surrounding the nanoparticles may influence the dielectric properties within nanocomposites [2, 7, 12, 13]

Due to the increment of the permittivity which was higher than other components of the polymer and the nanoparticles, an abnormal distortion of the electric field could occur in nanocomposite systems. A significant amount of water molecules affect nanoparticles and the interphase region, thus influencing the dielectric properties of nanocomposites, especially at low frequencies [18, 19]. The existence of high relative permittivity of the pure water, $\varepsilon r = 80$ [5] in the nanocomposites, percolation or sub-percolation paths could provide a path for enhanced the charge transfer process in nanocomposites [5]. This phenomenon could contribute to increased nanocomposites' conductivity, thus resulting in lower breakdown strength.

V. Conclusion

Two interphase models surrounding a nanoplatelet have been modeled and analyzed. The results showed that different permittivity values can either reduce or increase the electric field intensity in the resulting nanocomposites. As the permittivity values of the interphase region were varied, the electric field distribution of the interphase models were affected. If the permittivity value of the interphase fell between the polymer ($\varepsilon r \sim 2.3$) and the nanoplatelet ($\varepsilon r \sim 5.5$), the electric field in the resulting nanocomposite will be less distorted. However, as the permittivity value of the interphase became much higher (7.5) or lower (1.5), the electric field intensity became greatly distorted. It is noteworthy that the electric field intensity within the interphase region of the circularly-shaped interphase was found to be less distorted compared to the rectangular-shaped interphase model. Therefore, the presence of different interphases plays an important role in determining the electric field intensity of nanocomposites. Nevertheless, further experimental work needs to be carried out to extend the current understanding.

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References

[1] J. K. Nelson, "Nanodielectrics - The First Decade and Beyond," *Proceedings of 2014 International Symposium on Electrical Insulating Materials (ISEIM)*, 2014.

[2] S. Raetzke, and J. Kindersberger, "Role of Interphase on the Resistance to High-Voltage Arcing, on Tracking and Erosion of Silicone/SiO2 Nanocomposites," *IEEE Transactions Dielectrics And Electrical Insulation*, vol. 17, no. 2, pp. 607-614. 2010.

[3] K. Y. Lau, et al., "Polyethylene Nanodielectrics: The Effect of Nanosilica and Its Surface Treatment on Electrical Breakdown Strength," *Annual Report Conference Electrical Insulation and Dielectric Phenomena (CEIDP)*, 2012.

[4] P. Balagurusamy, et al. "Modeling and Behaviour of partial discharge in nanocomposite materials." *2014 International Conference on Circuit, Power and Computing Technologies (ICCPCT),* 2014.

[5] L. Hui, J. K. Nelson, and L. S. Schadler, "The Influence of Moisture on the Electrical Performance of XLPE/Silica Nanocomposites," *10th IEEE International Conference in Solid Dielectrics (ICSD)*, 2010.

[6] 6C. S. Daily, et al., "Modeling the Interphase of a Polymer-Based Nanodielectric," *IEEE Transactions Dielectrics And Electrical Insulation*, vol. 21, no. 2, pp. 488-496. 2014.

[7] K. Y. Lau, et al., "Modeling of Polymer Nanocomposites: Permittivity vs. Electric Field Intensity," *IEEE International Conference in Power and Energy (Pecon),* 2014.

[8] T. Andritsch, et al., "Modeling of the Permittivity of Epoxy Nanocomposite," *IEEE Conference In Electrical Insulation And Dielectric Phenomena (CEIDP),* 2013.

[9] M. Roy, et al., "Polymer Nanocomposite Dielectrics-The Role of the Interface," *IEEE Transactions Dielectrics and Electrical Insulation*, vol. 12, no. 4, pp. 629-643, 2005.

[10] T. Tanaka, et al., 'Proposal of a Multi-Core Model for Polymer Nanocomposite Dielectrics," *IEEE Transactions Dielectrics and Electrical Insulation*, vol. 12, no. 4, pp. 669-681. 2005

[11] M. Todd, and F. Shi, "Dielectric Characteristics of Complex Composite Systems Containing Interphase Regions in Advanced Packaging Materials: Processes, Properties And Interfaces," *9th International Symposium Proceedings*, 2004.

[12] 1D. Yan, et al., "The Influence of Interphase between Nanoparticles and Matrix on Youngs Modulus of Nanocomposites," *International Conference Nanoscience and Nanotechnology (ICONN)*, 2008.

[13] I. A.Tsekmes, et al. "Modeling the dielectric response of epoxy based nanocomposites," *2014 Electrical Insulation Conference (EIC)*, 2014.
[14] D. Fabiani, G. C. Montanari, and L. Testa, "Effect of aspect ratio and water contamination on the electric properties of nanostructured insulating materials," *IEEE Transactions on Dielectrics and Electrical Insulation,* vol.17, no. 1, pp. 221-230. 2010.
[15] J. K. Nelson, *Dielectric Polymer Nanocomposites*, Springer New York Dordrecht Heidelberg London, 2010.
[16] D. Pitsa, and M.G. Danikas, "Interfaces features in polymer nanocomposites: A review of proposed models," *Nano*, vol. 6, no. 6, pp. 497-508, 2011.
[17] I. L. Hosier, et al., "Effect of Water Absorption on Dielectric Properties of Nano-Silica/Polyethylene Composites," *IEEE Conference Electrical Insulation and Dielectric Phenomena (CEIDP)*, 2014.
[18] I. L. Hosier, A. S. Vaughan, and R. D. Chippendale, "Permittivity Mismatch and Its Influence on Ramp Breakdown Performance," *IEEE International Conference Solid Dielectrics (ICSD)*, 2013.