Effect of Interphase Region and Neighboring Particles on Electric Field Intensity within Nanocomposite Systems

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***Abstract*—Recent works show that the presence of the interphase surrounding nanoparticles can improve the dielectric properties of nanocomposites. Also, neighboring particles in the nanocomposites affect the electric field distribution. Therefore, the objective of this paper to model and analyze the effect of one-dimensional (1D) nanofillers towards the electric field distribution when the interphase and neighboring are taken into account inside the nanocomposite system. By using Finite Element Method Magnetics (FEMM) 4.2 software, a model of nanocomposites system consists of polymer matrix, nanoparticle filler with interphase and neighboring particles is modeled under the electrostatic problem module. Electric field intensity is observed with different distance between adjacent nanoparticles and interphase region permittivity values. The result obtained show that the presence of the interphase with various permittivity value will result in distorted electric field intensity surrounding a nanoparticle. Furthermore, the electric field intensity also affected when adjacent nanoparticles displaced between each other within nanocomposites.**

***Index Terms*—Electric Field Intensity; Interphase; Nanocomposites; Neighboring Particles; Permittivity.**

I. INTRODUCTION

Nanotechnology have grown in various applications such as in the field of electronics, electrical, bioengineering and material and mechanical engineering [1, 2]. The study of the nanostructure materials has been emerged for the past half century in terms of electrical, mechanical, thermal and other properties which can enhanced the polymer nanocomposite properties [1-5]. Polymer nanocomposites has been well known among researchers as it contains the combination of any nanofiller's shape with base polymer through blending process. The unique combinations of this materials promise the enhancement of the dielectrics properties on the electrical conductivity, breakdown behavior, treeing resistance, corona resistance, etc. All these have in [2-15] and this phenomena is now inviting interest among other researchers. Polymer nanocomposite also exhibits breakdown mechanism similar to pure polymer [16-18]. The presence of the interphases region (a layer between the polymers matrix and the nanofiller) and the neighboring nanoparticles are claimed can affect the material properties.

Many reports have been written on the properties of the interphase between nanoparticles and the polymer matrix that can influenced the nanocomposites system [6, 10, 11, 13, 19-23], however there are still lack of discussion and analyses that have yet to be revealed especially the effect of the neighboring particles in the polymer nanocomposite and the preposition of the interphase region. It is important to study the influence of the interphase and its affect towards the neighboring particles in the nanocomposite materials to the electric field distribution due to the interaction and interplay between nanoparticles remain unsatisfactory.

Therefore, this paper continuous to the previous work in [13] in order to clearly understand the role of the interphase in the nanocomposites study of the previous work focusing on the effects of the neighboring particles. The analysis of the effect of interphase and neighboring particles on the electric field distribution is achieved by modeling one-dimensional (1D) nanofiller as nanoparticle filler in polymer matrix by using Finite Element Method Magnetics (FEMM) 4.2 software.

II. MODELING AND PARAMETERS DESCRIPTION

The dimensions of the design in the FEMM 4.2 software under electrostatics model were initialized by using a simple polymer slab with thickness of 1 µm and width of 2 µm, placed between 10 kVdc High Voltage (HV) potential and 0 V ground potential, as shown in Figure 1.

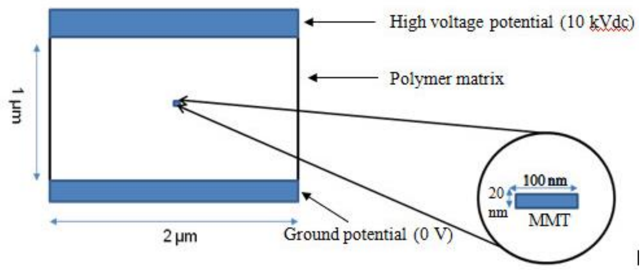

Figure 1: A two dimensional slab with thickness 1 µmand width 2 µm was placed between 10 kV DC high voltage (HV) potential and 0 V ground potential.

As a starting point, all of the designs were accomplished by using specific permittivity value for the polymer matrix and the nanoparticle filler. Based on the literature review, polyethene with dielectric permittivity, εr = 2.3 [9, 24, 25] was selected as the polymer matrix while the chosen (1D) nanofiller was montmorillonite nanoclay (MMT) with εr=5.5 [26]. For analyze the effect of the interphase region and neighboring nanoparticles, the information above was considered for all subsequent modeling. Meanwhile, the theoretical model of the spherical interphase region surrounding one-dimensional (1D) nanofiller with discrete thickness based on 'water shell' that has been emphasized and highlighted by Davide Fabiani et al., the ideal of the spherical region obtained by consider the rotation around the centers and it is possible in the case of the one-dimensional (1D) nanofiller such as fluorohectorite, montmorillonite nanoclay etc [27]. As the exact value of the interphase permittivity still unknown, the interphase permittivity value was varying from 1.5, 3.5, 5.5 and 7.5 (case B1, B2, B3 and B4) in order to investigate it effect to the electric field intensity within nanocomposite system. The details of the model materials are presented in Table 1. An example of the electric field distribution within nocomposite with separation distances 100 nm apart from the nanoparticles surface between the neighboring nanoparticles as shown in Figure 2.

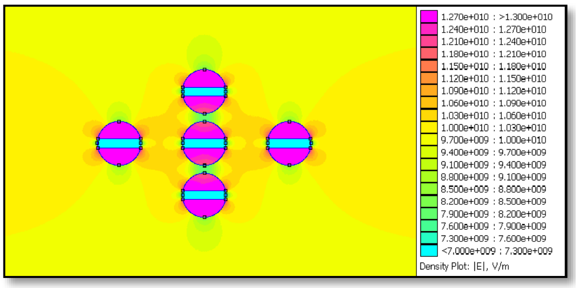

Figure 2: Electric field distribution a nanocomposite with neighbouring nanoparticles with separated 100 nm apartHV) potential and 0 V ground potential.

Table 1
Details of the polyethylene, montmorillonite nanocalays and interphase properties

Material	Size	Permittivity
Polymer (PE)	Slab (1μm x 2μm)	2.3
Nanoparticle (MNT)	Platelet (20nm x 100nm)	5.5
Interphase	Circular with 50 nm in radius	Varying values (between 1.5 to 7.5)

Before the result is discussed, it reasonable to assumed 5 situations in this section, as following situations, i.e.,

i. The separation distances between the neighboring particles is 0 nm
ii. The separation distances between the neighboring particles is 40 nm
iii. The separation distances between the neighboring particles is 80 nm
iv. The separation distances between the neighboring particles is 100 nm
v. The separation distances between the neighboring particles is 180 nm

III. RESULTS AND ANALYSIS

Platelet nanoparticles were permitted to touch each other with neighboring nanoparticles when the nanoparticles filler was loaded at higher concentrations and beyond this high loading of nanoparticles, it fall under Situation I; separated 0 nm between two neighboring nanoparticles. Figure 3 shows the effect of electric field intensity of a nanocomposite containing two neighboring nanoparticles separated 0 nm apart (Situation I). From Figure 3, it can be seen that when permittivity value of the interphase was lower (1.5) than other components (polymer and nanoparticle), the electric field intensity between lines A1 and B1 is enhanced. However, outside line B1 and outwards, lower permittivity of the interphase cause to deep electric field intensity sags below the unfilled polymer. An opposite effect can be observed for the case of higher permittivity value of the interphase (case B4). Whilst, the models perform better fit data for the permittivity values of interphase that were laid between the polymer and nanoparticle which were less distorted than the cases discussed earlier. At the same time, similar pattern has been obtained for case A and B3 with extreme suddenly changes of electric field intensity at line A1 and B1, respectively. Besides, it is observed that when analyze on line B1 outwards from the interphase surface, the electric field become less distort and maintain at one level known as unaffected polymer within nanocomposite [20].

A present nanometric radius of interphase region around the platelet nanoparticles may provide an area of overlap interphase region with neighboring interphase. A model of nanocomposite (represent as Situation II) and its effect on the electric field intensity are shown in Figure 4. As the distance between the two adjacent neighbouring nanoparticles was separated at 40 nm (Situation II) which is interphase region begins to overlap as depicted in Figure 4.

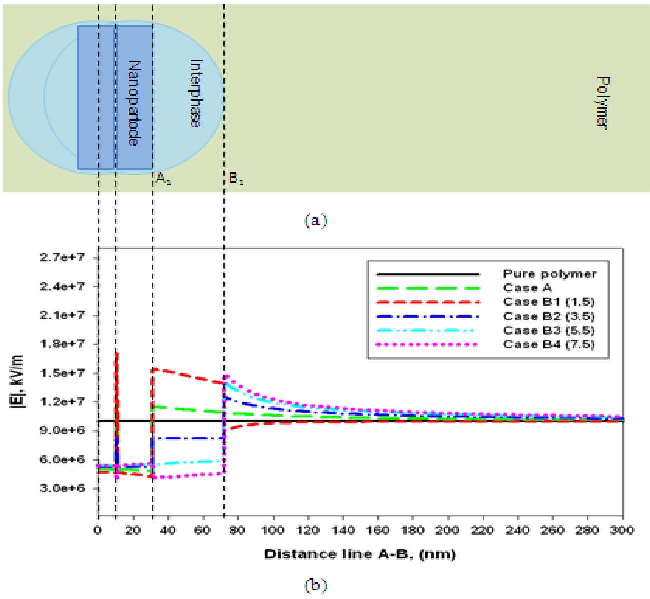

Figure 3: Effect of (a) nanoparticle (with separated 0 nm apart) on the (b) plots of the electric field intensity along the line AB from the origin

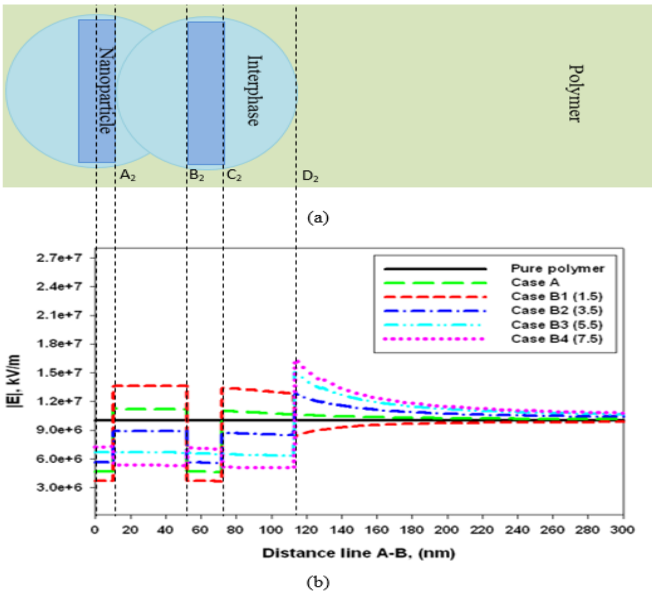

Figure 4: Effect of (a) nanoparticle (with separated 40 nm apart) on the (b) plots of the electric field intensity along the line AB from the origin

As the nanofiller loading was reduced in the polymer, the area overlap of interphase region will be decreasing. There is no overlap occurred however the surface of the interphase touching each other with the neighboring nanoparticles as shown in Figure 5 (separated 80 nm between two nanoparticles). This situation is defined as Situation III. The advantage of having an interphase permittivity value between polymer (2.3) and nanoparticle (5.5) for case B2 becomes visible as the distortion of the electric field intensity became lower than the unfilled polymer by analyzing line A3 to line D3. Overall, case B2 show electric field intensity having less distortion compared to the model having no interphase and permittivity value of interphase similar with nanoparticle (case B3), lower (case B1) and higher (case B4) than other components. Furthermore, the electric field intensity was decreasing between lines A3 to C3 compared with Situation II.

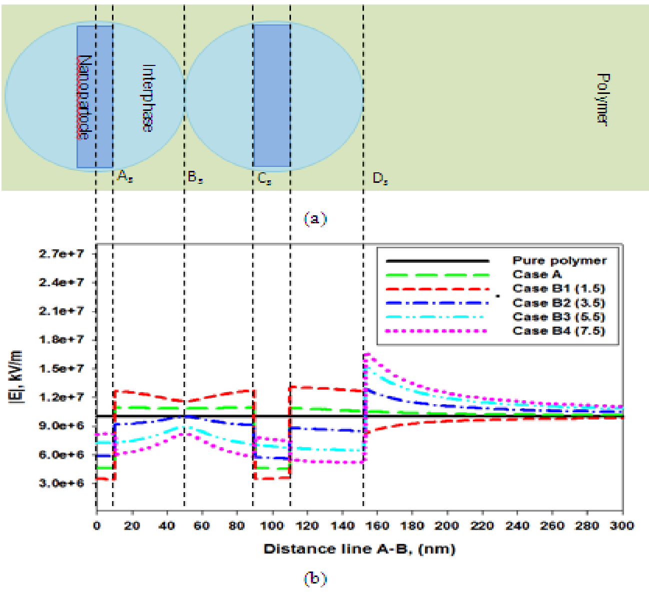

Figure 5: Effect of (a) nanoparticle (with separated 80 nm apart) on the (b) plots of the electric field intensity along the line AB from the origin

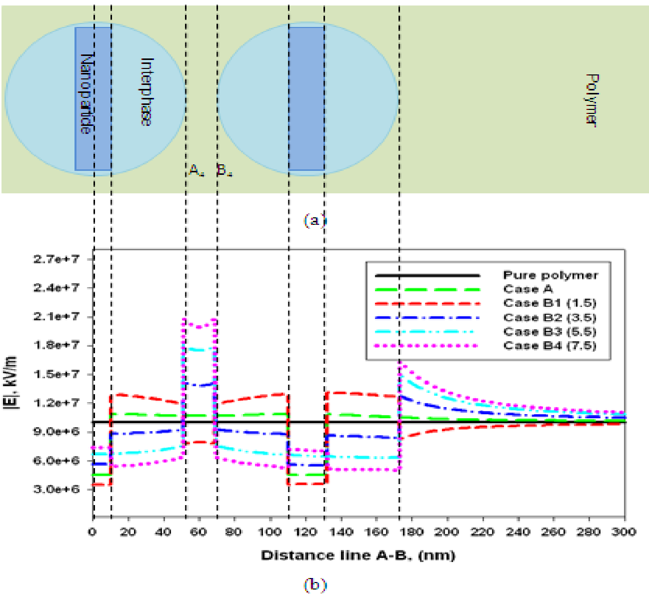

Figure 6: Effect of (a) nanoparticle (with separated 100 nm apart) on the (b) plots of the electric field intensity along the line AB from the origin

Within the nanocomposites with low nanofiller loading, it is expected that no interphase overlap and separated by a distance between the interphase surface of neighboring nanoparticles mark as Situation IV as shown in Figure 6 (separated 100 nm between two nanoparticle). It is observed that the electric field intensity distributes more variables between lines A4 and B4 by comparing each cases of having an interphase region (case B1, B2, B3 and B4). Within this region (between lines A4 and B4), high permittivity value of interphase region (case B4) than other components was observed to have very high of electric field intensity (~2.0x107 kV m-1) as compared to other regimes. Whilst, the electric field intensity shows sign of increment for cases B2 and B3 when compare with the electric field distribution as shown in Figure 5(b).

Within the nanofiller loading are relatively very small the surface of the interphase between neighboring nanoparticles detached with the greater distance, as shown in Figure 7 (separated 180 nm between two nanoparticles). This condition indicates as Situation V. This final regime seems like similar with Situation IV, however the difference was between the distances between neighboring nanoparticles which has been separated further away. The pattern of the electric field distribution in Figure 5(b) has given the similar effect compared to the Figure 4(b) however the effect can be observed more shallow between lines A5 and B5 when the separations between the neighboring nanoparticles was more further increased. By analyzing between line A5 and B5, the maximum value of electric field intensity was slightly higher (~1.6x107 kV m-1) for higher permittivity value of interphase region (case B4) than other components but lower when compared to Figure 4(b). Furthermore, the electric field intensity seems to be less distorted for the case A and B1 as analysis start from the origin to outwards.

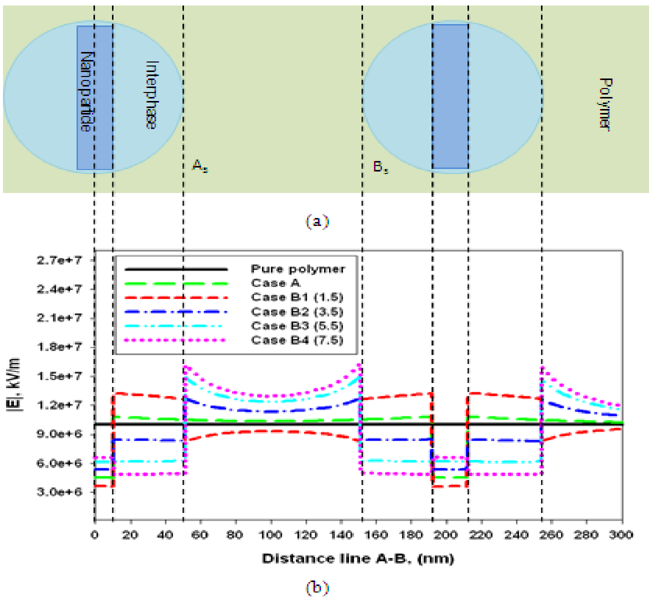

Figure 7: Effect of (a) nanoparticle (with separated 180 nm apart) on the (b) plots of the electric field intensity along the line AB from the origin

IV. Discussion

The increment of the permittivity which is higher than other components of the polymer and the nanoparticles, leads to abnormal distortion of the electric field which occurs in the nanocomposite systems. This can be clarified by the mechanisms presence of water. Water, oxygen and other can also be absorbed onto the surface the nanoparticle during the manufacturing process and a layer is formed between the nanopaticles and the polymer [18, 28, 29]. These phenomena contribute to enhance conductivity in nanocomposites and results in lower its breakdown strength.

The lower permittivity of the materials will result in interfacial polarization mechanism in the bulk within the nanocomposites becomes limited [6, 21, 30].This modeling predicts the anomalous maximum electric field intensity would occur within the nanocomposites with large distortion when permittivity value of the interphase region lowers than other components. With high and large distortion of electric field, this might reduce breakdown performance within this high field region. Meanwhile, this research results indicates the permittivity value in the interphase region should in between the polymer ($\varepsilon r \sim 2.3$) and the nanoparticles ($\varepsilon r \sim 5.5$) appears as it reduces the electric field intensity within the nanocomposite systems and this opposite effect to the previous research reported for permittivity in the interphase region [11, 13].

On the other hand, another reason affecting the electric field intensity in resulting nanocompasites is due to the neighboring nanoparticle. Basically, the overlapping of the interphase region and the distance separation between two neighboring nanoparticle depend on the nanoparticles volume fraction and the shape and size of the nanoparticles [21]. As filler nanoparticles concentration increases, the possibility of the nanoparticles touch each other and the region surrounding each nanoparticle known as interphase region might be begin to overlap and vice versa. Indirectly, these cases can affect the electric field distribution in resulting nanocomposites considering the neighboring nanoparticle.

As aforementioned, at higher permittivity values, the interphase region between nanoparticles and polymer matrix might be deboneded by the presence of water. This molecule presence during the production of the materials due to the effect temperature and humidity surrounding. In the real environment, this phenomenon describes on how the “water shell” model was built up in nanocomposites. These conditions emphasized when sufficient water injects into the interphase region, the interphase region around the nanoparticles might have a quasi-conductive (QDC) as the interphase region overlapping each other’s [23, 29]. This QDC provide the paths for the charges and carriers at higher amount of montmotillnite (MNT) nanoparticles, shorter separation between the neighboring nanoparticles and lower temperature at low frequency. Thus, this subsequently leads to high electric field and resulting in lower breakdown strength.

V. CONCLUSION

The presence of an interaction zone known as the interphase region has been claimed as one of the significant role that can affect the dielectric properties. The distribution of the electric field is observed to have different distortion due to the variation in permittivity value of the interphase and can also be due to the influence of the presence of a neighboring nanoparticle. Furthermore, electric field intensity within the nanocomposites can have reduce and increment based on the permittivity value of the interphase region and the loading of nanofillers. Thus this analysis explained the exhibit breakdown performance and understanding about breakdown strength in resulting nanocomposites system by considering of the interphase region and neighboring nanoparticles.

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