Simulation of the Effects of Nano-filler Interactions in Polymer Matrix Dielectric Nanocomposites

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Abstract

Polymer matrix dielectric composites with high permittivity and low loss can be used as potential materials for high energy density electrical energy storage [1,2], piezoelectric generators [3] and electromechanical transducers[4] and other applications. Many theoretical models have been developed for predicting the dielectric properties of polymer-matrix composites[5]; however, none of them can explain and/or predict the experimental results when there are complexities in the microstructure. Therefore, finite element simulations that take the arrangement of the nanofillers as well as their size and distribution into consideration have been conducted in order to improve dielectric property predictions. A polymer matrix filled with spherical nanofillers was used as a model system in a 3D configuration.

Dielectric polarization and relaxation mechanisms in polymer matrix nanocomposites can be largely affected by the charge storage behavior of ferroelectric nano-fillers and/or the charge transport behavior of conductive nano-fillers. The impedance response of dielectric composites was calculated in the frequency domain using the AC/DC Module of the COMSOL Multiphysics® software. Dielectric properties were calculated from the impedance data[6].

The objective was to solve the quasi-static form of Maxwell's equations for the electric potential and electric displacement in the 3D geometry. Nano-sized fillers with different properties, size, morphologies and orientations were used in the simulation to describe the interactions between fillers. Figure 1(a) shows a schematic of the simulation configuration and geometry. Figure 1(b) shows a calculated electric displacement field map of a composite containing 47.9 vol % barium titanate (BT) nanoparticles (NPs). Figure 2 shows the effects of inter-particle distance of nanoparticles on the electric displacement field. The electric displacement in between 2 adjacent nanoparticles increased by more than 2.2 times as the inter-particle distance decreased from 60 nm to 10 nm when the particle size was 78 nm. A schematic in figure 2 (b) shows that the interaction zone becomes stronger as the inter-particle distance decreases. In other words, it can be expected that the interaction will be greater the higher the filler concentration is [7].

It was found that when the filler concentration exceeded 20%, it was necessary to include the interaction fields proposed by Jaysundere and Smith [8], in order to predict the dielectric properties more accurately. Simulation and experimental results will be reported for BT filled composites as a function of concentration and interaction field size. The developed simulation model is applicable to many different types of nanocomposite systems, because this model is based on the real geometric arrangement of nano-fillers

and their properties which is one of the most important factors in determining the effective permittivity of composite materials.

Reference

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Figures used in the abstract

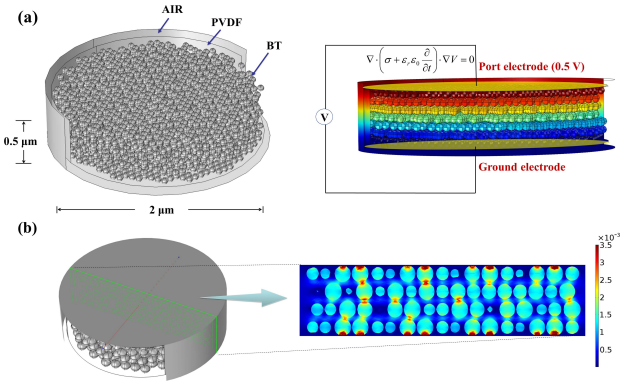

Figure 1: (a) Schematic of the configuration for dielectric simulation and (b) calculated electric displacement field map of a composite containing 47.9 vol % barium titanate (BT) nanoparticles (NPs).

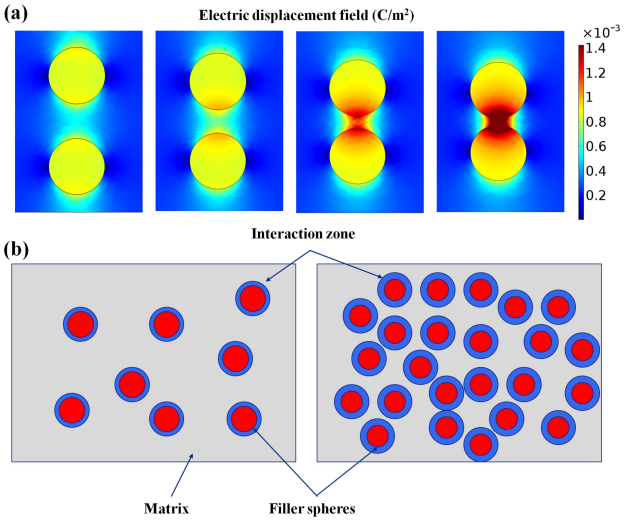

Figure 2: (a) Effects of inter-particle distance in electric displacement field in between BT NPs (60, 40, 20, and 10 nm from the left) and (b) Schematic of interaction zone with respect to inter-particle distance; image redrawn from ref [7].