Modeling and Simulation of High Permittivity Core-Shell Ferroelectric Polymers for Energy Storage Solutions

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Abstract

Extensive interest is being invested into the research of polymer based nanodielectrics. Such a material provides a more practical energy storage solution primarily for embedded capacitors. Polymer embedded metal nanofiller is considered as a great choice to achieve the above stated high energy storage. Our earlier simulation work reported that capacitors fabricated with dielectrics consisting of Au (core) and SiO2 (shell) nanocomposites, dispersed in Polyvinyl Pyrrolidine (PVP) polymer solution, showed a maximum electrical permittivity K of 2600 at 10kHz with 0.16% nanoparticles loading. The K values were calculated using effective medium theories (EMT) of Maxwell-Garnett, Bruggeman and Looyenga models. However, the experimental findings with similar loading showed very low K values. This is because the simulation results were based on highly ordered nanoparticles in the polymer matrix, a configuration which is quite difficult to achieve experimentally. We propose to narrow this discrepancy in the results by developing nanodielectric films based on embedding highly ferroelectric Polyvinilydine fluoride (PVDF) polymer matrix with high conductivity aluminum (Al) cores and solid aluminum oxide (Al2O3) as capping shells for electrical insulation and simulate the system considering less ordered nanoparticles in polymer matrix to feedback the experimental work. This approach is simple, cost effective and employs a polymer which is chemically inert to most solvents. It is also a low smoke generation material during a fire event which makes it possible to use in embedded capacitor applications. Apart from the above features, it is highly ferroelectric which adds up in further enhancing the dielectric response at lower applied electrical fields with a minimum amount of nanoparticle loading. In COMSOL Multiphysics® software, the AC/DC Module is selected and the in plane electric currents are applied to the physical model. The modified EMT with equations representing the ferroelectric nature of the polymer is applied to the polymer core-shell to calculate the effective electrical properties of the composite. The percolation data analysis is used to predict the maximum theoretical K value of the nanocomposite and results of both 2D and 3D models under different amount of filler loading will be presented.