Prediction Of Electro-elastic Properties Using COMSOL Multiphysics For Energy Harvesting Domain

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Abstract

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In this work, the positive enhancing effect of conductive polyaniline (PANI) as an interfacial core-shell layer coated over a piezoelectrically active barium titanate (BTO) nanoparticles on the output electro-elastic properties (relative dielectric constant, piezoelectric co-efficient, and elastic modulus) of a polyurethane polymer nanocomposite is predicted employing a modified Eshelby-Mori-Tanaka micromechanics (EMT) methodology. Finite element analysis (FEA) methodology based on kinematic uniform boundary conditions (KUBC) has been employed to verify the accuracy of the modified EMT-based micromechanical model. The relative dielectric constant (k/k_0) values of various BTO(PANI) core-shell composites as identified from the literature are also compared with our EMT-model-based predictive data.
The influence of PANI over the final effective electro-elastic output of the polyurethane nanocomposite has also been evaluated as a function of BTO volume fraction and PANI interfacial layer thickness. In addition, the mixed aspect ratio for the multiparticle core-shell polymer matrix composite, which has particle size and aspect ratio distribution corresponding to the microstructural analysis of commercially procured BTO nanoparticles is elaborated. The effect of different BTO filler aspect ratios for multiparticle mixed aspect ratio BTO filler was also studied separately for EMT and FEA models having variable conductive PANI interfacial layer thickness (50 nm and 75 nm).
The modified EMT micromechanics methodology in our study is capable of effectively capturing the enhancing effect of the PANI interfacial layer on the output electro-elastic properties with increasing BTO filler concentration and PANI shell thickness. The predicted effective electro-elastic output properties as obtained from the modified EMT-based micromechanical analysis are also observed to be a good match with FEA-based predictive output. Multiple three-phase composites identified from the literature are also compared to be a close match to our EMT micromechanics methodology-based predictive output.
These predictive results and interpretation of data for 0-3 polymer matrix composite having BTO(PANI) core-shell layer is a representative first step towards the design of effective nanogenerators of multi-phase core-shell inclusion geometry. The micromechanical methodology employed in this work also sheds light on the key role of the positional arrangement for filler and interfacial layer within the matrix phase in the prediction of effective properties that are effectively being captured in FEA based prediction model. This work can also be expanded to complex microstructural geometry considering the random orientational alignment of the inclusion (filler and interphase) geometries.

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