

Modeling of Bipolar Charge Transport through Nanocomposite Films for Energy Storage

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Abstract : The effects of ferroelectric nanofiller size, shape, loading, and polarization, on bipolar charge injection, transport, and recombination through amorphous and semicrystalline polymers are studied. A 3D particle-in-cell model extends the classical electrical double layer representation to treat ferroelectric nanoparticles. Metal-polymer charge injection assumes Schottky emission and Fowler-Nordheim tunneling, migration through field-dependent Poole-Frenkel mobility, and recombination with Monte Carlo selection based on collision probability. A boundary integral equation method is used for solution of the Poisson equation coupled with a second-order predictor-corrector scheme for robust time integration of the equations of motion. The stability criterion of the explicit algorithm conforms to the Courant-Friedrichs-Levy limit. Trajectories for charge that make it through the film are curvilinear paths that meander through the interspaces. Results indicate that charge transport behavior depends on nanoparticle polarization with anti-parallel orientation showing the highest leakage conduction and lowest level of charge trapping in the interaction zone. Simulation prediction of a size range of 80 to 100 nm to minimize attachment and maximize conduction is validated by theory. Attached charge fractions go from 2.2% to 97% as nanofiller size is decreased from 150 nm to 60 nm. Computed conductivity of 0.4×10^{14} S/cm is in agreement with published data for plastics. Charge attachment is increased with spheroids due to the increase in surface area, and especially so for oblate spheroids showing the influence of larger cross-sections. Charge attachment to nanofillers and nanocrystallites increase with vol.% loading or degree of crystallinity, and saturate at about 40 vol.%.

Keywords : nanocomposites, nanofillers, electrical double layer, bipolar charge transport

Conference Title : ICPMSE 2015 : International Conference on Polymer Materials Science and Engineering

Conference Location : Venice, Italy

Conference Dates : November 09-10, 2015