Effect of Matrix Plasticizing Conditions and Filler Interfacial Properties on the Percolation Threshold of Polymer-Carbon Composites

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Critical amounts (percolation threshold) of conducting fillers such as carbon black (CB), metal particles, or carbon fibers blended with an insulating polymer can be used to achieve dielectric properties for both fundamental and applied interests in sensing applications. The dependence of the percolation threshold on carbon filler surface conducting properties and conditions for matrix plasticization by solvent(s) is complicated. We report an experimental and theoretical approach based on molecular modeling to evaluate the effect of carbon filler interfacial properties and solvent conditions for polymer matrix plasticization on the percolation threshold of the polymer-carbon composites. For the current study poly(4-vinylphenol) and polyethylene oxide polymers are considered for the composite formation. The carbon fillers investigated include carbon black (Cabot Black Pearls 2000) and graphite whiskers, which differ in surface area, surface functionality and conductivity. The film resistivities as a function of carbon loading are evaluated. The results will be evaluated to determine the percolation threshold for varying filler interfacial properties and polymer solvent plasticizing conditions (solvent polarity and compositions). Molecular modeling will be used to provide insights based on filler-filler, matrix-matrix, and matrix-filler interactions.

Keywords: Polymer-carbon composite, Percolation threshold, Plasticizing conditions, Molecular modeling