Influence of Factors affecting the Percolation Curve of Polymer-Carbon Composites on Electronic Nose Response

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The Electronic Nose (ENose) sensor developed at JPL for environmental monitoring in a crew habitat of a spacecraft uses arrays of polymer-carbon black composite sensing films. The optimum weight percentage of conducting filler that is blended with the insulating matrix polymer is critical in achieving dielectric properties in order to get a stable sensor response. The percolation curve of polymer-carbon composite is affected by many factors including carbon filler surface conducting properties, conditions for matrix plasticization by solvent(s), polymer morphology (crystalline vs. amorphous nature) and the molecular weight of the polymer.

We report an experimental and molecular modeling based theoretical approach to evaluate the influence of polymer matrix plasticizing conditions as well as filler interfacial properties on the percolation curve of the polymer-carbon composites. The polymers under consideration for the composite formation include poly(4-vinylphenol), polyethylene oxide (100K and 1000K MW) and ethyl cellulose. 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 curve for varying filler interfacial properties and polymer solvent plasticizing conditions (solvent polarity and compositions). The polymer composite films will then also be tested for their selectivity, sensitivity and stability of response to detect acetone and isopropanol.

Molecular modeling strategies will be used to provide an insight for the percolation studies by calculating the filler-filler, matrix-matrix, and matrix-filler interactions as well as composite-analyte interactions. Predicted composite-analyte interactions will also be compared to sensor response to validate the molecular model.

Keywords: Electronic Nose, Polymer-carbon composite, Percolation curve, Molecular modeling