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Cellular Automata Simulations of Thermal and Electrical Transport Properties of Thin-Film Polymer/CNTs Nanocomposites ALEX CASEY, Assumption College, GERMANO IANNACCHIONE, Worcester Polytechnic Institute, GEORGI GEORGIEV, Assumption College and Tufts University, PEGGY CEBE, Tufts University — A computational algorithm has been developed to simulate the transport properties of oriented and un-oriented thin film nanocomposites of isotactic Polypropylene (iPP) and carbon nanotubes (CNT) with increasing CNT concentration. Our goal is to be able to design materials with optimal properties using simulations. We use cellular automata approach in Matlab simulation environment. The percolation threshold is reproduced in the simulations, matching experimental data. Upon percolation, the thermal transport in the films increases sharply, more so for the electrical than for the thermal conductivity, due to the larger difference in the electric conductivities of the CNTs and the polymer. To verify the simulation, the thin-film samples were sheared in the melt at 200 C at 1 Hz in a Linkan microscope shearing hot stage. The thermal and electrical conductivity measurements were performed on the same cell arrangement with the transport perpendicular to the thin-film plane using a DC method. The thermal and electrical conductivity are higher for the un-sheared as compared to the sheared samples with stronger temperature dependence for the latter as compared to the former. Our cellular automata simulations provide information about the microstructure-macroscopic property relation in the thin film nanocomposites and can be extended to simulations of other important materials.

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