 Proceedings of ICCES'08, pp.1237-1237

A Complex Network Based Simulation for the Electric Characterization of Nanocomposites

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Summary

It is well known that the addition of conducting fillers to a polymeric matrix can result in a significant improvement of its electrical and mechanical properties. Although the electrical properties of heterogeneous composites have been widely investigated in the past years, the electrical properties of composites containing carbon nanofibers are not sufficiently understood.

In recent years, the need to study real networks systems like the Internet, social networks and biological systems has resulted in a variety of techniques which can be used in the context of material science simulations.

Under the framework of complex networks, one can make use of several distributions, such as connectivity and centrality. These distributions, together with others parameters that can be extracted from the network (graph diameter, cluster coefficient), can help relate the electrical properties and behavior with the underlying structure of the composite material. Simultaneously, these methods open the possibility of relating computational results to experimental ones.

In order to explore the potential application of complex network methods to nanocomposites, we constructed a computer model that employs the Graph theory to represent a physical system. From the virtual models of nanofiber networks dispersed in dielectric polymeric matrices and by applying the boundary element method to numerically solve an electro-quasistatic problem, we build a weighted network.

In this paper we present our model and, by selecting some case studies, we show the behavior of distributions and parameters in the selected cases. Namely, our approach enables us to evaluate the system response to the removal of the higher centrality value node, classify the type of network, or identify clustering effects.

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