



Complex networks to simulate electrical properties in disordered materials

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Abstract – In this work we propose a new perspective to study electrical conductivity in the disordered materials based on complex networks as the Erdős-Rényi and Scale-free networks. The theoretical results are similar to experimental results obtained from semiconducting polymers, such as polyaniline. Both results indicated that interchain processes govern the resistivity behavior in the low-frequency region while, for higher frequencies, intrachain mechanisms are dominant. The model intends to take the inherent inhomogeneity of scale-free networks to take into account the structure aspects of a semiconducting polymer, and simulate the transport mechanisms in disordered materials.

Complex networks are currently being studied across many fields of science. Undoubtedly, many systems in nature can be described by models of complex networks, which are structures consisting of nodes or vertices connected by links or edges. In fact, many systems around us display rather complex topologies, that often seem random and unpredictable. For example, the cell, a network of chemicals linked by chemical reactions, and the Internet, a network of routers and computers connected by physical links. Thus, the conduction process regarding the electrical conductivity in disordered materials has been widely considered by researchers in experimental and theoretical environments, in such a way that diversity of morphological structures assumes that carrier charge process may behave as intramolecular and intermolecular process. The alternating conductivity technique is an appropriate tool not only to identify, but also to quantify the contributions of each process. Therefore, the simulations of alternating conductivity and conduction processes involved in disordered materials are able to support the understanding of properties in materials. In this work we propose a new perspective to study electrical conductivity in the disordered materials based on complex networks as the Erdős-Rényi and Scale-free networks. The conduction processes are simulated on a (random and scale-free) network composed by electrical circuits. The circuits are formed by resistors and capacitors in parallel associations become related with the displacement current or only resistors associated with the conduction current. Capacitances and resistances are randomly attributed following some statistical distribution. The source terminals in the complex network are based on the intuitive notion of peripheral and central regions proposed as two different load modes. In the first load mode the source terminal is applied between the central and the periphery terminal while in the second the source terminal is applied between P1 and P2 (the two halves of the peripheral region). In this work we investigated the some parameters (as nodes and links number) on the simulation of the electrical properties from disordered materials yet. The results indicated that the electrical properties can be simulated by a statistical model based on complex networks. The theoretical results are similar to experimental results obtained from semiconducting polymers, such as polyaniline. Both results indicated that interchain processes govern the resistivity behavior in the low-frequency region while, for higher frequencies, intrachain mechanisms are dominant. The model intends to take the inherent inhomogeneity of scale-free networks to take into account the structure aspects of the real polymer, and simulate the transport mechanisms in disordered materials.

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