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Simulated electrical response of randomly distributed and aligned graphene/polymer nanocomposites

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Abstract. *In this work, a recently developed numerical method that simulates the electrical response of a graphene/polymer nanocomposite is validated with experimental data. The approach is based on the multiscale method and consists of a unit cell and a representative volume element (RVE), accounting for aligned and randomly distributed nanoparticles. At the unit cell level, the material nano characteristics (filler geometry, constituent electrical and interfacial properties) are integrated into a local resistance algebraic matrix. The material architecture is then modelled at the micro-level (RVE) by a user-defined distribution of the unit cell electrical properties. A statistical sample was studied and the average electrical response was compared with measurements for direct (DC) and alternate current (AC). The proposed methodology accurately describes the nanocomposite electrical behaviour with its volume fraction and loading frequency. The model is proven to be an effective, flexible and time-efficient tool to design and optimize advanced nanocomposite systems.*

Keywords: Nano-structures, Polymer, Graphene, Percolation Threshold, Finite Element Analysis (FEA), Computational modelling, Electrical Properties, Electrical Conductivity

1 Introduction

1.1 Background

Conductive polymers are considered for their potential applications in light emitting devices, batteries, electromagnetic shielding and piezoresistive sensors. In literature, there are several material systems proposed, including all the possible combinations of insulating polymer and conductive nano-micro-particle, such as carbon black [1-2], metallic powder [3–5], polyaniline [6], MWCNTs and graphite [7]. Great attention has also been paid to polymers reinforced by graphene and its derivatives, due to progress in their manufacturing process and attractive thermal and electrical behaviour [8–15].]. The effect of the multilayer graphene thickness and temperature on electrical conductivity was studied in [8], while the impact of synthesis on electrical performance was explored by studying compacts of graphene [9], graphene oxides produced by different synthesis routes [10] and reduced graphene oxides [11]. In [12], reinforcing polymer with graphene resulted in significant improvement of the thermal performance, while the thermal transport was studied for free-standing graphene nanoribbon as a function of temperature [13], and for suspended graphene sheets with different sizes [14]. Large-area reduced graphene oxide thin film was fabricated and examined by the authors in [15] that showed improved electrical and thermal conductivity with enhanced electromagnetic

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