3D Percolation Modeling for Predicting the Thermal Conductivity of Graphene-Polymer Composites

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Abstract

Graphene-based polymer composites exhibit a microstructure formed by aggregates within a matrix with enhanced thermal conductivity. We develop a percolation-based computational method, based on the multiple runnings of the shortest path iteratively for ellipsoidal particles to predict the thermal conductivity of such composites across stochastically-developed channels. We analyzes the role of the shape and the aspect ratio of the flakes and we predict the onset of percolation based on the density and particle dimensions. Consequently, we complement and verify the conductivity trends via our experiments by inclusion of graphene aggregates and fabrication of graphene-polymer composites. The analytical development and the numerical simulations are successfully verified with the experiments, where the prediction could explain the role of larger set of particle geometry and density. Such percolation-based quantification is very useful for the effective utilization and optimization of the equivalent shape of the graphene flakes and their distribution across the composite during the preparation process and application.

Keywords: Composite Polymer, Percolation, Elliptic Fillers, Thermal Conductivity.

1 Introduction

Polymer composites with augmented thermal conductivity values are promising materials with potential applications in industries such as electronics and renewable energy systems [1, 2]. Polymers have very low in-plane thermal conductivity with less than $0.2 W/m/K$ for polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) [3], therefore the insertion of highly conductive graphene

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