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PAPER

Multiscale modelling of thermal conductivity of carbon nanotube paraffin nanocomposites

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Abstract

Paraffin waxes can store large amount of heat according to their high heat capacity, which is a high quality property to address some fundamental concerns in technology, like the thermal management of rechargeable batteries. The thermal conductivity of paraffin is rather low, which can be improved by changing their chemical composition or by adding additional components. In this regard, one solution is to fabricate nanocomposites structures through adding nanofillers to paraffin. Carbon based nanostructures such as carbon nanotubes offer among the highest thermal conductivities available in the nature. Therefore, they could be considered as the best candidates to enhance the heat conduction of paraffin. In this study we developed multiscale modelling to investigate the thermal conductivity of CNT/paraffin nanocomposites using a combination of atomistic and continuum approaches. For this purpose, molecular dynamics simulations were carried out for the assessment of the thermal conductance between the CNT and paraffin at nanoscale. We evaluated the thermal conductivity of CNT/paraffin by the means of finite element method. We finally studied the effects of volume fraction and geometric parameters of fillers on the effective thermal conductivity of CNT/paraffin nanocomposites. Our findings in this study provide good vision regarding managing the thermal conduction in CNT/paraffin nanocomposite.

1. Introduction

It is quite well-known that paraffin waxes with the structure including long chain hydrocarbons, can absorb large amount of heat according to their high capacity [1, 2]. Like a heat sink, they can store high amount of heat while their temperature nearly remains constant [3]. According to their applications, there are various types of paraffin waxes that each of them is applicable for certain temperature ranges. The thermal properties of paraffin waxes can be changed by altering their chemical composition or by adding additional fillers [4, 5]. One of the most important applications of paraffin is for the thermal management of lithium ion batteries (LiBs). LiBs currently play critical roles in electricity supply and power reservoir [6]. Continues request due to technological developments throughout the last decade for wireless communications, handheld electronics and electric cars have emerged the interest for LiBs [7, 8]. It should be noted that the thermal conductivity of paraffin is rather low which is not desirable for the application in the thermal management systems. Carbon based nanostructures such as the graphene [9–11] and carbon nanotubes [12] offer the highest thermal and mechanical properties available in the nature [13–20]. Therefore, they could be considered as the most promising candidates to enhance heat conduction of paraffin. Recent experimental studies have confirmed that adding graphene and CNT to commercial paraffin can enhance the thermal conductivity of the mixture [21–28]. In addition there exist some computational efforts to simulate and predict the enhancement of thermal properties of paraffin by adding nanoparticles [29–34].

The objective of this study is therefore to investigate the thermal conduction in CNT/paraffin nanocomposites. To this aim, we will develop multiscale model using classical molecular dynamics and finite