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Thermal transmittance of carbon nanotube networks: Guidelines for novel thermal storage systems and polymeric material of thermal interest

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ABSTRACT

Among other applications, the study of thermal properties of large networks of carbon nanoparticles may have a critical impact in *loss-free*, more compact and efficient thermal storage systems, as well as thermally conducting polymeric materials for innovative low-cost heat exchangers. In this respect, here, we both review and numerically investigate the impact that nanotechnology (and in particular carbon-based nanostructures) may have in the near future. In particular, we focus on the role played by some geometrical and chemical parameters on the overall thermal transmittance of large complex networks made up of carbon nanotubes (CNTs), that can be potentially added as fillers to (thermally) low-conductive materials for enhancing the transport properties. Several configurations consisting of sole and pairs of single-walled carbon nanotubes (SWCNTs) and double-walled carbon nanotubes (DWCNTs), characterized by different dimensions and number of C–O–C interlinks, are considered. Based on the results found in the literature and using focused simulations using standard approaches in Non-Equilibrium Molecular Dynamics (NEMD), we highlight the dependence on the particle diameter, length, overlap and functionalizations of both thermal conductivity and boundary resistance across CNTs, which are indeed the relevant quantities for obtaining composite materials with desired unusual thermal properties. We observe that CNTs with short overlap length and a few interlinks already show a remarkable enhancement in the overall transmittance, whereas further increase in the number of C–O–C connections only carries marginal benefits. We believe that much understanding has been gained so far in this field thanks to the work of chemists and material scientists, thus it is time to draw the attention of engineers active in the energy sector and thermal scientists on such findings. Our effort, therefore, is to gather in this article some guidelines towards innovative thermal systems that may be manufactured and employed in the near future for addressing a great challenge of our society: Storage and use of thermal energy.

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1. Introduction

Thermal energy storage for sufficiently long periods is known to be a critical issue in thermal sciences. In general, nanotechnology (and particularly carbon based nanostructures) may hold the premise for successfully addressing energy issues in modern society [1,2].

In particular, recently, an innovative system with the capacity of storing thermal energy potentially for an indefinite time have attracted much attention thanks to the pioneering work of scientists at the Fraunhofer Institute for Interfacial Engineering and Biotechnology, together with ZeoSys GmbH [3]. In addition, such a new technology can store three to four times more energy compared to water based systems. The new system contains zeolite pellets and one of the key challenge here is (i) to ensure optimal heat transfer (high overall conductivity) through the zeolites during the thermal loading and (ii) to allow water percolation during the thermal release, in the same device. The latter competing (and extreme) features may be met by dispersing highly conductive materials (fillers) within the zeolite pellets (matrix) [4].

The use of carbon-based nanoparticles (e.g. carbon nanotubes, graphene, etc.) certainly represents one of the most promising alternative. On the other hand, even for perfectly dispersed fillers forming an ideal percolating network, realizing a sufficiently high thermal transmittance for the overall network is everything but a simple task. In fact, typically high thermal resistances are experienced by the heat flux across the several interfaces characterizing such composite materials (see e.g. [5,6]). It is therefore highly desirable to systematically investigate on the several mechanisms that contribute to the value of the overall thermal transmittance of such complex percolating networks. Moreover, those studies have a critical impact also on polymeric materials for innovative heat exchangers and other composite materials [7–10].

Since their first observation by Iijima [11], Carbon Nanotubes (CNTs) have attracted an increasing attention because of their outstanding physical properties. In fact, superior mechanical, electric and (most importantly) thermal properties of CNTs have been reported [12], and this certainly makes such material a versatile building block for future engineering applications [13].

Among others, thermal properties of CNTs have been widely investigated in recent years, both experimentally and theoretically [14,15]. For instance, pristine CNTs are characterized by one of the largest value of thermal conductivity, ranging from 2400 $W\,m^{-1}\,K^{-1}$ to 4740 $W\,m^{-1}\,K^{-1}$ depending on the experimental conditions [14]. Moreover, thermal conductivity of CNTs may be tuned by introducing defects, vacancies, surface functionalizations or junctions [16,17], thus allowing the design of CNT-based composite materials with desired enhanced thermal properties [18,19]. CNT-based composites are typically made out of polymeric, ceramic or metallic matrices and carbon-based fillers, such as CNTs, graphene or carbon nanoribbons [20,21].

CNTs spontaneously tend to bundle and cross-link each other because of their high intermolecular cohesive forces [22], whereas precise geometries of CNT networks can be induced by means of proper chemical functionalizations [23]. Therefore, CNT networks are energetically and thermodynamically stable up to 600 K, and CNTs synthetized within a polymeric or ceramic matrix can exist in a stable and designable cross-linked form [24]. Due to their peculiar thermal and technological properties, CNT fillers have been employed in a promising variety of applications, such as thermal interface material [25–27], electrical interconnects [28], electronic nanocircuits [29], triggered drug release [30], artificial muscles [31], thermal nanocircuits [32–34], nanofluids for heat transfer [35–37], energy harvesting [38] and gas or thermal storages [24,39]. For example, CNT networks are promising technological solutions for improving the internal distribution of heat within thermal storage applications, such as nanoporous zeolite devices, in order to reach a better control and efficiency of the heat accumulation/release cycle [40]. In the latter case, CNT networks need to be engineered and properly designed for reducing thermal losses at low filling ratio in the matrix. However, experimental benchmarks and molecular simulations of carbon-based networks reveal an overall thermal performance lower than expected, which is mainly due to CNT–CNT and CNT–matrix thermal boundary resistances [41–44].

It is well known that heat conduction by CNTs is predominantly a phononic phenomenon (i.e. coupled vibration of carbon atoms), rather than an electronic one [45]. The reasons for high thermal conductivity of CNTs are due to their large speed of sound, long range crystallinity and long phonon mean free path [14,46]. Nevertheless, the bottleneck of heat transfer within carbon-based networks is the thermal boundary resistance (also known as Kapitza resistance), which defines the thermal impedance between different materials. Kapitza resistance is generated by phonon scattering, which produces a local temperature discontinuity in heat transfer phenomena at the nanoscale. Vacancies, functionalizations, defects as well as interfaces between different materials (solid or liquid) contribute to thermal boundary resistance [47–55]. Therefore, the difference between intertube and intratube thermal conduction, which can also be orders of magnitude, limits the overall thermal transmittance of the CNT-based composites. Hence, a better understanding of the geometry, chemistry and arrangement of CNT networks is needed, in order to have guidelines in designing composite materials with desired heat transfer performances. Recent studies about carbon-based composite materials show that a better efficiency in heat transfer is achieved when CNTs percolate within the matrix, creating a homogeneous and cross-linked network [6,56,57]. Owing to the current experimental difficulties in synthetizing high quality and well-ordered CNTs, computational studies have been conducted to systematically analyze the thermal properties of CNT and CNT networks [57–60]. Among others, Molecular Dynamics (MD) simulations have been widely used for improving the physical understanding and predicting the thermal transport in carbon-based composite materials [61]. In this study, thermal properties of CNTs with different diameter, length, chirality, number of walls, overlap and chemical functionalization are investigated by means of MD simulations. Hence, this work aims at systematically reporting and analyzing the geometrical and chemical parameters affecting the thermal conductivity and the thermal boundary resistance of CNT networks, in order to come up with a few general guidelines for designing the overall thermal transmittance of CNT-based composites.

2. Materials and methods

Non-Equilibrium Molecular Dynamics (NEMD) simulations are performed for estimating the thermal conductivity λ of CNTs and the thermal boundary resistance R_k between adjacent CNTs. The latter configuration can be regarded as the building block of large