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Thermal interface tailoring in composite materials

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ABSTRACT

The thermal transport in heterogeneous materials systems, such as in composites, is essentially controlled by the phonon scattering phenomena at the materials interface due to the interface materials property mismatch. Such phenomena are also prevalent in joints or component interfaces. The thermal property mismatch at the materials interface, in the molecular scale, is primarily dictated by the phonon density of state across the interface. In this paper, the interface materials configuration for tailoring the thermal properties of composite materials with nano constituents is presented. The materials modeling using both the finite element analysis (FEM) and molecular dynamics (MD) simulations is performed to identify the effect of materials constituent scale as well as the nano constituent surface functionalization on the interface thermal transport phenomena. It is observed that the effect of surface functionalization towards establishing covalent bonding between the nano constituent surface the matrix (such as polymers) is extremely important in enhancing the interface thermal conductance.

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1. Introduction

Nonmetallic (polymeric) composites, because of its weight advantage over its metallic counterpart, are extensively used in printed circuit board to aerospace systems. In addition, in view of managing the excess thermal loads generated by the thermal devices in aerospace systems, there is an increasing emphasis of tailoring thermal transport properties of composite materials. The anticipated pay-off of improving the thermal properties of composites is primarily in the significant weight savings for the aerospace systems, as compared to the metallic materials. In the carbon fiber reinforced polymeric composites, continuous carbon fibers (either in the laminated or woven form) are embedded in the polymer matrix. The axial thermal conductivity of carbon fibers is known to be quite high; ranges from 20 W/m-K (for Pan carbon fiber) to 1000 W/m-K for pitch carbon fiber (for example, 900–1000 W/m-K for Thornel® K1100 pitch fiber). Thus, the in-plane thermal conductivity of carbon fiber composites (the plane containing the fiber axis) varies between 10 W/m-K to 500 W/m-K, which is significantly high as compared to its transverse conductivity (less than 1 W/m-K). A primary reason of the poor transverse (perpendicular to the fiber axis) thermal conductivity of composites is due to the fact that the fibers are embedded in a polymeric matrix phase, which is primarily insulative (whose thermal conductivity is the range of 0.2–0.3 W/m-K). Furthermore, the phonon scattering due to the existence of significant impedance mismatch at the interface between the fiber and the matrix is also contributes to the reduction of its transverse thermal conductivity.

In order to make the polymer matrix composites viable to thermal applications, it is through thickness (i.e., perpendicular to the fiber axis) thermal conductivity needs to be significantly enhanced. Thus, it is logical to introduce a conductive phase in the matrix to facilitate thermal pathways to overcome this deficiency. There has been numerous study of dispersing CNTs in polymers to enhance the thermal conductivity of the polymeric phase [1–3]. But, the improvement was very limited, only up to 120%, which does not meet any of the application requirements mentioned earlier. The primary reason of this very limited improvement in the conductivity is due to the phonon scattering at the CNT–polymer interface caused by the enormous acoustic mismatch between CNT tips and polymer [4]. Thus, terminating the CNT tips in the polymer is not a viable option for significantly enhancing thermal conductivity in composites, through the polymer phase.

The through-the-thickness (i.e., perpendicular to the fiber direction) thermal conductivity (K_z) of this type of materials, even with the modification of the matrix with conductive nano fibers (Fig. 1) is in the order of 1–1.5 W/m-K, which fails to meet the thermal performance requirements in microelectronics, space, and propulsion applications. A current survey of space and propulsion community revealed a value of K_z of about 10 W/m-K will enable lean manufacturing of space structures and significant weight savings for thermal management in propulsion structural components [5,6]. The primary reason of the very limited improvement (up to ~1–1.5 W/m-K) is the termination of the conductive nano fibers in the polymer matrix, which causes the

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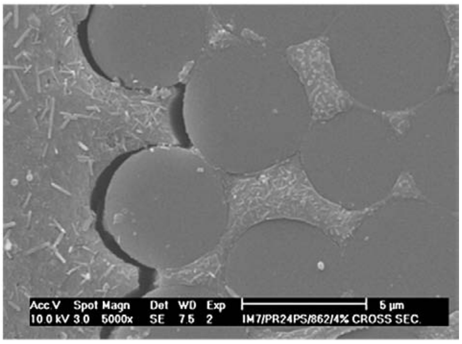

Fig. 1. The plane of the micrograph represents transverse direction to the fiber axis of carbon fiber (IM7) polymer composite. The matrix modified with carbon nano fibers. The thermal conductivity (K) of the composite along the plane of the micrograph is measured to be around 1.2 W/m-K.

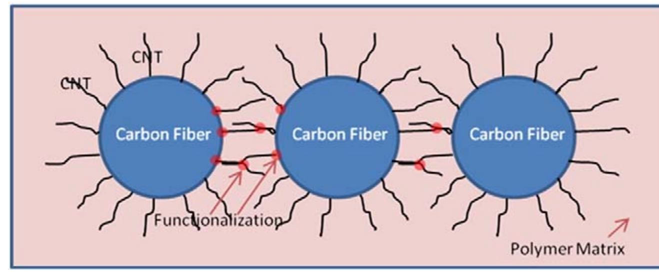

Fig. 3. A schematic view of the hierarchical carbon fiber composite. Sufficiently long CNTs grown on carbon fiber form the intermingled network embedded in the polymer matrix to provide the thermal pathways through the matrix phase.

phonon to scatter at the interface between the nano fiber tips and the polymer. Thus, a possible way of significantly enhancing the transverse thermal transport in the polymer matrix composites is to establish a conductive pathway through the polymer matrix phase between the adjacent fibers. The conductive pathway could possibly be established by incorporating the carbon nano tubes making the connections between the carbon fibers through the matrix. Thus, conductive carbon nano tubes (CNTs) grown on the carbon fiber surface with appropriate surface functionalization to make CNT–CNT contact is expected to establish such pathway through the matrix phase. Similarly, in the case of bonded joints, the incorporation of CNTs aligned along the thickness direction with CNT tips making the thermal contact with the adherent surface (i.e., by establishing the thermal interface between the CNT tips and the adherent surface) provides the promise of enhancing the through-thickness thermal conductivity in the bonded joints. The key to the success of the above mentioned two concepts relies essentially on establishing the appropriate interface thermal contact.

1.1. Hierarchical hybrid carbon fiber concept for composites

The hierarchical carbon fiber materials morphology of conductive carbon nano tubes (CNTs) grown on the carbon fiber surface potentially may provide thermal pathways through the matrix phase. The CNTs of sufficient length should be grown on carbon fibers so that the CNTs form an intermingled and connected network embedded in the matrix phase for facilitating the thermal pathways through the polymer matrix. Such effort has recently been carried out several researchers, including Zhang et al. [7]. The representative micrographs of CNTs grown on carbon fibers (the hierarchical carbon fiber morphology) of such effort are shown in Fig. 2. These hierarchical hybrid carbon fibers are then to be infused with polymer to form the composites. In order for this hybrid carbon fiber composite to form the above mentioned network of conductive pathway through the polymer phase, the CNT tips or CNT side walls to make thermal contact with the adjacent CNTs. The thermal contacts of the adjacent CNTs possibly can be achieved through appropriate surface functionalization. A schematic view of this concept is shown in Fig. 3.

In order to understand the feasibility of this concept, the thermal conduction by means of a finite element analysis (FEM) of a unit cell representing the hexagonal array of carbon fibers with CNTs anchored on its surface was performed, Fig. 4. In this two-dimensional FEM, it is assumed that adequate density of CNTs are grown throughout the fiber surface such that the CNTs are considered to behave as thin plates with its plane aligned along the fiber axis. The FEM analysis (Fig. 4) revealed that the CNT intermingled network (i.e., continuous CNT pathway between the adjacent fibers through the matrix) is essential. In addition, the increasing the transverse thermal conductivity of the carbon fibers is also a big factor in enhancing the overall thermal conductivity of the composite in the direction perpendicular to the fiber axis. The pan-based carbon fibers do not possess good thermal conductivity, due to its amorphous microstructure—thus is not preferred in thermal composites. The conductive pitch-based carbon fibers (for example, Thornel® K1100, etc.) provide excellent conductivity along its axial direction. In addition, the radial graphene microstructure in pitch-based carbon fibers is known to offer attractive transverse thermal conductivity, Fig. 5. The above observation made through the finite element calculation, as shown in Fig. 4, is based on the assumption of perfect CNT–fiber and CNT–CNT interface thermal contact (i.e., there is no thermal resistance between the CNT–fiber and CNT–CNT interface). The validity of such assumption depends on how well such interface is established. An assessment of such interface performance and the feasibility of establishing such interfaces will require molecular level modeling, which will be discussed later in Section 1.3.

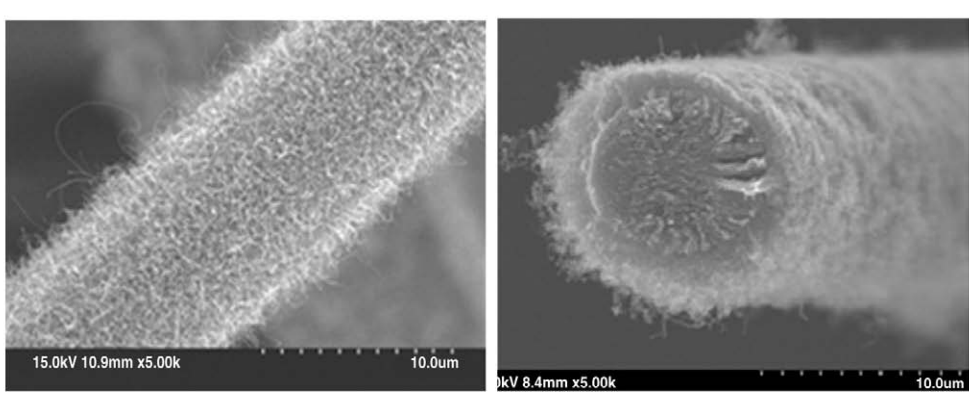

Fig. 2. Micrographs of hybrid carbon fiber (CNTs grown on carbon fiber surface).