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The percolation threshold for tensile strength of polymer/CNT nanocomposites assuming filler network and interphase regions

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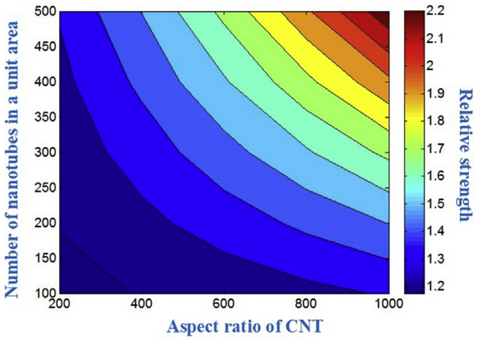
HIGHLIGHTS

- Percolation threshold for tensile strength of polymer/CNT nanocomposites is studied.
- Filler network is a strengthening agent in PCNT beside the interphase.
- The suggested equations are applied in some samples and the results are explained.
- The effects of several parameters on the strength of PCNT are discussed.

GRAPHICAL ABSTRACT



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ABSTRACT

In this article, the percolation threshold for tensile strength of polymer/CNT nanocomposites (PCNT) is studied by known Pukanszky model. Since the network of nanoparticles forms at very low concentration of CNT, the filler network shows strengthening efficiency in PCNT beside the interphase regions surrounding nanoparticles. The Pukanszky model is developed by the properties of network such as density (N) and strength (σ_N). The suggested equations are applied in some samples and the results are explained. Also, the effects of several parameters such as "N", "σ_N" and percolation volume fraction (ϕ_p) on the strength of PCNT are plotted based on the developed model. The direct influences of "N" and "σ_N" as well as the inverse effect of "ϕ_p" on the tensile strength of PCNT are displayed. The "σ_N" parameter only changes the strength of PCNT at low "ϕ_p", which shows the important role of percolation level.

1. Introduction

Among the nanoparticles, carbon nanotubes (CNT) are good candidate and excellent reinforcement for polymer nanocomposites. The CNT consist of thin and long graphite layers with diameters of 1–100 nm and lengths of 1–10 μm. Moreover, CNT are conducive filler with the high Young's modulus of about 1 TPa (1000 GPa) and the good tensile strength of 10–50 GPa [1–5]. As a result, CNT show remarkable physical properties such as high aspect ratios and large surface area, exceptional mechanical behavior and noble conductivity, which cause the CNT to be a promising reinforcement in advanced nanocomposites [6–8].

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During the synthesis of nanocomposites, the van der Waals attraction between CNT forms the aggregates and agglomerates. So, it is vital to break the aggregates/agglomerates and afford the good dispersion of nanotubes in the polymer matrix to improve the mechanical properties. In fact, good dispersion of CNT in polymer matrix is necessary to achieve the desirable mechanical performance in nanocomposites [9,10]. Also, the high interfacial area and the strong interfacial interaction/adhesion between polymer matrix and nanoparticles forms a third phase as interphase which significantly affects the mechanical properties of polymer nanocomposites [11–13]. The interphase properties mainly depend on several parameters such as polymer characteristics, dispersion and surface treatment of CNT, interfacial interaction, etc. [11,12]. The molecular interaction at the interphase determines the efficiency of stress transfer from polymer to nanofiller. The properties of interphase such as thickness, strength and modulus have been well studied in polymer nanocomposites by different models in the literature [14–16]. The significant reinforcement of nanoparticles in the nanocomposites was shown by formation of a thick and strong interphase between polymer matrix and nanoparticles.

The percolation threshold is the minimum content of nanofiller in the nanocomposite, which forms the filler network and produces an acceptable conductivity. So, the polymer/CNT nanocomposites (PCNT) display the electrical conductivity when the volume fraction of CNT is greater than the percolation threshold [17,18]. Beside the conductivity, a similar percolation was reported for mechanical properties of polymer nanocomposites by adding the filler concentration [19–21]. Researchers studied the mechanical percolation experimentally and theoretically. The electrical and mechanical percolations are consistent in PCNT, while the abrupt increase of mechanical behavior can be hardly explained by the mechanism of electrical percolation threshold [22]. It should be noted that the tensile strength of PCNT weakens at high filler concentrations, due to the aggregation/agglomeration of nanoparticles and stress concentration [23], while the electrical conductivity and tensile modulus improve upon increasing of CNT content. This issue is the main difference between tensile modulus and strength of nanocomposites and thus the theoretical bases for these properties are quite different.

Many authors in the literature have applied the models to study the electrical conductivity of PCNT by percolation effect [24–26]. Also, the role of percolation threshold in the tensile modulus of polymer nanocomposites was also reported. The conventional models cannot predict the percolation threshold in the polymer nanocomposites, because they cannot consider the unusual properties of nanofillers such as high aspect ratio, big surface area and networking above a certain concentration. Ouali et al. [27] developed a conventional model for tensile modulus of conventional composites by the percolation threshold. Researchers estimated the tensile modulus of polymer nanocomposites above percolation threshold by Ouali model [28,29]. However, the researches in this area should continue to suggest the models, which can take into account the properties of nanoparticles and its network above percolation threshold.

The percolation threshold in which the filler network forms was inversely related to the aspect ratio of nanoparticles [22,30]. Thus, the high aspect ratio of CNT produces the nanoparticles network in PCNT at very low filler concentrations. In this paper, the known and valid Pukanszky model is applied to investigate the percolation threshold for tensile strength of PCNT. The significant strength of polymer nanocomposites was attributed to the formation of interphase between polymer and nanoparticles. However, the tensile strength of some PCNT is higher than the predictions of the Pukanszky model in the highest levels of interphase thickness and strength. As a result, the high level of strength of PCNT is due to the percolation effect and the formation of CNT network above percolation threshold. The properties of network such as density and strength are assumed in a parameter as "B_N" which is determined in some samples by Pukanszky model. Also, the effects of network properties on the "B_N" parameter and tensile strength of PCNT are plotted and explained. By the suggested equations and the experimental results of tensile strength, it is possible to approximate the properties of interphase and filler network, when their influences on the strength of PCNT are certain. In fact, we try to present a simple approach for modeling of tensile strength in nanocomposites by considering the interfacial status between nanofiller and polymer matrix as well as the CNT networks above percolation threshold.

2. Model analysis

The Pukanszky model [31] for tensile strength of polymer nanocomposites containing well-dispersed nanoparticles (good dispersion of nanoparticles in polymer matrix is considered in this study) is expressed as:

$$\sigma_R = \frac{1-\phi_f}{1+2.5\phi_f}\exp\left(B\phi_f\right) \tag{1}$$

where "σ_R" is relative strength as the strength of nanocomposite per the matrix strength. Also, "ϕ_f" is filler volume fraction and "B" considers the capacity of stress transfer between the phases as an interfacial parameter. The Pukanszky model has been successfully applied for different polymer nanocomposites in the previous studies [31,32]. The "B" parameter depends on the thickness and strength of interphase as:

$$B = \left(1 + A_c d_f t\right)\ln\left(\frac{\sigma_i}{\sigma_m}\right) \tag{2}$$

where "σ_m" is the tensile strength of polymer matrix and "A_c" and "d_f" show the specific surface area and density of nanofiller, respectively. Also, "t" and "σ_i" are the thickness and strength of interphase. Therefore, the "B" parameter can be applied to characterize the properties of interphase in polymer nanocomposites. Both "t" and "σ_i" depend on the interfacial interaction/adhesion between polymer matrix and nanoparticles [33,34]. The strong interfacial interaction such as chemical bond causes thick and strong interphase, which can accelerate the percolation of CNT and improve the mechanical properties of PCNT. However, the low levels of "t" and "σ_i" negatively affect the networking of CNT and the mechanical behavior of nanocomposites.

The Pukanszky model can be restructured to:

$$\ln(\sigma_{Reduced}) = \ln\left(\sigma_R\frac{1+2.5\phi_f}{1-\phi_f}\right) = B\phi_f \tag{3}$$

where the plot of ln ($\sigma_{Reduced}$) against "ϕ_f" results in a linear correlation whose slope determines the "B" parameter.

The "A_c" parameter can be expressed for nanocomposites containing well-dispersed CNT as:

$$A_c = \frac{A}{m} = \frac{2\pi Rl}{d_f\pi R^2 l} = \frac{2}{d_f R} \tag{4}$$

where "A" and "m" are the surface area and mass of CNT, respectively. Also, "R" and "l" are the radius and length of nanoparticles. By replacing of "A_c" from above equation into Eq. (2), the "B" parameter can be expressed as: