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A model for tensile strength of polymer/carbon nanotubes nanocomposites assuming the percolation of interphase regions

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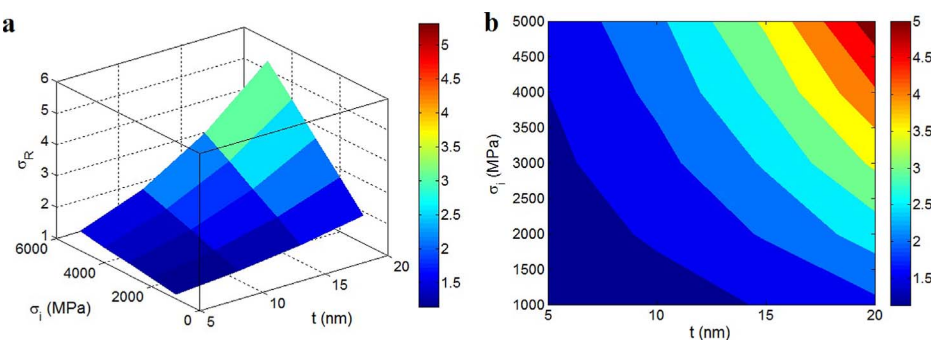
GRAPHICAL ABSTRACT



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ABSTRACT

In this paper, a model is developed for tensile strength of polymer/carbon nanotubes nanocomposites (PCNT) assuming the network formation above percolation threshold based on Ouali approach. The reinforcing and networking roles of interphase are also considered in the developed model, because the interphase regions commonly form in polymer nanocomposites. Several equations are established to enable the developed model to predict the strength using the properties of polymer matrix, nanoparticles, and interphase. The suggested model is evaluated using the experimental results of several samples. Also, the logical and average levels of thickness, strength, and percolation threshold of interphase regions are calculated for the reported samples. The developed model shows acceptable agreement with the experimental results of nanocomposites. Additionally, the developed model demonstrates the reasonable effects of the volume fraction and radius of nanoparticles as well as the volume fraction, percolation threshold, thickness and strength of interphase on the strength. All observations validate the predictability of the developed model for tensile strength of PCNT.

1. Introduction

The outstanding mechanical, thermal, electrical, and magnetic properties of carbon nanotubes (CNT), as well as their low density, low cost, large surface area, and chemical stability have motivated numerous researchers to focus on polymer CNT nanocomposites (PCNT) [1–4], because they can be applied in electronics, sensors, electromagnetic and durable products [5–7]. CNT possess a Young's modulus around 1000 GPa, as well as tensile strength of 11–50 GPa, producing very desirable mechanical and electrical performance [8]. CNT can also

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provide a conductive network that transfers charge and converts insulated polymer matrices into conductive nanocomposites [9,10]. However, aggregation of CNT due to intrinsic van der Waals attraction weakens their dispersion and deteriorates the mechanical and physical properties of PCNT [11,12]. Many physical and chemical methods have been suggested to solve this problem, such as chemical functionalization of CNT, dispersion of CNT in a polymer solution by sonication, and in-situ polymerization with CNT [13]. It has been reported that modification of the CNT surface by functionalization of acidic groups is an effective method of forming a uniform dispersion of CNT in a polymer matrix [13,14].

The percolation point is the smallest volume fraction of nanofiller making the continuous network within the matrix [3,15]. A percolation threshold is commonly observed in nanocomposites where a conducting nanofiller (such as CNT) is added to a polymer matrix, because the electrical conductivity profoundly increases at this point changing the insulating matrix into a conductive sample. Interestingly, the percolation threshold was also reported for mechanical properties of polymer nanocomposites such as modulus, which is known as mechanical percolation [16–19]. Favier et al. [16] correlated the high values of shear modulus in composites containing cellulose whiskers to the percolation threshold of the filler. The models of mechanical percolation are commonly dependent on the electrical percolation. Ouali et al. [20] suggested a model using an inverse rule of mixtures to determine the tensile modulus of polymer composites containing a filler network. The connection between electrical and mechanical percolation may be true, because it was suggested that both of these occurrences for CNT are inversely related to the filler aspect ratio [21]. However, mechanical percolation has been concisely studied in polymer nanocomposites using experimental and theoretical approaches rather than relying on a correlation with electrical percolation.

Large surface area per volume and a high number density of nanoparticles commonly create an intermediate phase between the polymer matrix and nanoparticles, known as interphase, which is different from both the matrix and nanoparticles. Previous authors have extensively investigated the interphase specifications using experimental and theoretical approaches [22,23]. Some theoretical studies have focused on the micromechanics models for mechanical properties such as Halpin-Tsai and Tandon-Weng, expanding them by considering the interphase [24,25]. Some authors have experimentally demonstrated the presence of interphase regions in nanocomposites [26]. Furthermore, the formation threshold of a percolating network may be shifted to a lower volume fraction of nanoparticles due to the connection of interphase regions around the nanoparticles, termed pseudo-percolation [27,28]. This phenomenon shows good agreement with the predicted and experimental percolation thresholds in nanocomposites [29]. Nevertheless, pseudo-percolation has been studied only briefly in the literature.

In this study, a model is developed based on Ouali approach for tensile strength of PCNT, assuming the effect of percolation threshold. Since the interphase commonly forms in PCNT, the reinforcing and percolating roles of interphase are also assumed in the developed model. The suggested model can predict the tensile strength of PCNT using the properties of the polymer matrix, nanoparticles, and interphase. The developed model is evaluated using the experimental results of samples from previous articles, and the influences of all parameters on the predicted strength are debated.

2. Development of model

Ouali et al. [20,30] developed the inverse rule of mixtures to determine the tensile modulus of composites based on the percolation effect as:

$$E = \frac{(1-2\psi+\psi\phi_f)E_mE_f + (1-\phi_f)\psi E_f^2}{(1-\phi_f)E_f + (\phi_f-\psi)E_m} \quad (1)$$

where ϕ_f is volume fraction of filler, and E_m and E_f are the tensile moduli of polymer matrix and filler, respectively. Likewise, $\psi$is correlated to the volume fraction of percolation (ϕ_p) as:

$$\psi = 0 \quad \phi_f \le \phi_p \quad (2)$$

$$\psi = \varphi_f\left(\frac{\varphi_f-\varphi_p}{1-\varphi_p}\right)^b \quad \phi_f > \phi_p \quad (3)$$

where b is an exponent equal to 0.4 in a three-dimensional (3D) system [20]. Also, setting $\psi = 0$ below the percolation threshold reduces the Ouali model to the inverse rule of mixtures as:

$$E = \frac{E_mE_f}{(1-\phi_f)E_f + \phi_fE_m} \quad (4)$$

The Ouali model can be developed for the tensile strength of polymer nanocomposites because its origination is based on the inverse rule of mixtures. However, nanoparticle strength is not considered in models of tensile strength, because it results in overprediction of the strength of the nanocomposite. The stress is transferred from the polymer matrix to nanoparticles through the interphase regions. As a result, the interphase properties control the strength of polymer nanocomposites, because a poor interphase leads to nanoparticle debonding from the polymer matrix, deteriorating the role of nanoparticles [31]. By this reasoning, the strength of interphase plays a much larger role in the strength of PCNT than the strength of the nanoparticles. On the other hand, the interphase plays a significant role in stiffening and percolation, as discussed. The reinforcing effect of interphase is considered by assuming an additional phase surrounding the nanoparticles in the model. This is justifiable, as the interphase forms around the nanoparticles within nanocomposites. The percolating role of interphase is taken into account by the modified equation for percolation threshold.

So, when the interphase is considered in PCNT, the Ouali model is developed for tensile strength as:

$$\sigma = \frac{(1-2\psi+\psi\phi_f+\psi\phi_i)\sigma_m\sigma_i + (1-\phi_f-\phi_i)\psi\sigma_i^2}{(1-\phi_f-\phi_i)\sigma_i + (\phi_f+\phi_i-\psi)\sigma_m} \quad (5)$$

$$\psi = (\phi_f+\phi_i)\left(\frac{\phi_f+\phi_i-\phi_{pi}}{1-\phi_{pi}}\right)^{0.4} \quad (6)$$

where ϕ_i and σ_i are the volume fraction and tensile strength of interphase, respectively. Also, ϕ_{pi} is the percolation volume fraction of interphase regions. When the effects of filler and interphase are neglected, i.e., $\phi_f = \phi_i = 0$, the model calculates the strength of the polymer matrix.

Some equations are expressed with regard to the volume fraction and percolation threshold of interphase regions. The volume fraction of interphase in nanocomposites containing cylindrical nanoparticles (such as CNT) is stated [32] by:

$$\phi_i = \phi_f\left[\left(1+\frac{t}{R}\right)^2 - 1\right] \quad (7)$$

where R is the radius of nanotubes and t is interphase thickness.

The percolation threshold of cylindrical fillers [33] can be also suggested by:

$$\phi_p = \frac{V}{V_{ex}} \quad (8)$$

where V and V_{ex} are the volume and excluded volume of nanoparticles, respectively. The excluded volume is the volume around an object into which the center of a similar object cannot enter. The V and V_{ex} for a random distribution of spherically-capped cylindrical rods [34] are