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Modeling approach for tensile strength of interphase layers in polymer nanocomposites

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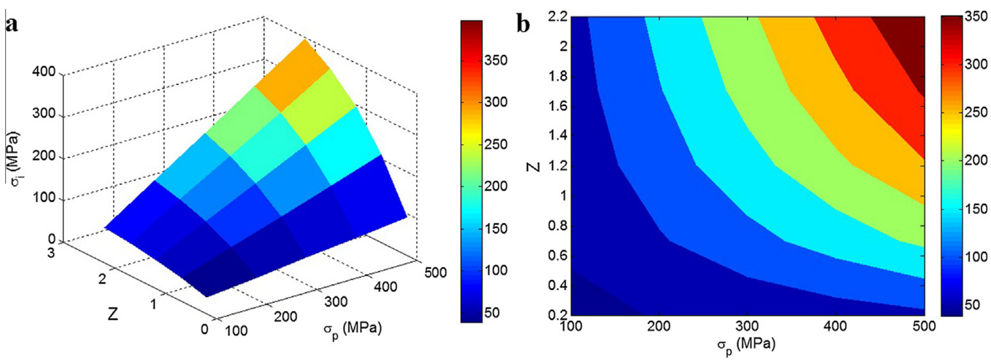
GRAPHICAL ABSTRACT



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ABSTRACT

At the first step, this paper describes a developed model for tensile strength of interphase layers (σ_k) in polymer nanocomposites. The "σ_k" is expressed as linear, exponential and power functions of the distance between nanoparticles and polymer matrix (x_k). Afterwards, the predictions of these equations at the central layer of interphase (the average strength) are compared to the calculations of interphase strength (σ_i) by several micromechanical models including the developed Leidner-Woodhams and Pukanszky models to choose the best equation which expresses "σ_k".

The calculations are carried out for several reported samples. The equation which expresses the "σ_k" as a power function of "x_k" shows the best results compared to others. Also, its predictions significantly depend to an exponent as "Z" which demonstrates the level of interphase properties. According to the chosen equation, the "σ_m" and "σ_p" play positive roles in "σ_i" predictions at low "Z" value, but a high "Z" eliminates the effect of "σ_m" on the tensile strength of interphase layers.

1. Introduction

The highly improved properties of polymer nanocomposites are achieved in low nanofiller content by a low-cost, easy and accessible method [1–6]. On the other hand, the addition of nanoparticles is much preferred because the high content of micro-particles significantly worsens the properties of the polymer matrix such as processability, appearance, weight and aging. Therefore, the desirable aspects of polymer nanocomposites vindicate the much work performed in this field [7–10].

Several main challenges restrict the development of polymer nanocomposites such as the uniform dispersing of nanofillers in the polymer matrix and also, providing a good interfacial adhesion between nanoparticles and matrix [11]. In the recent years (from

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1990s to now), the researchers have tried to obtain a better dispersion of nanoparticles in polymer matrix and promote the interfacial interaction in the polymer nanocomposites [12–14]. In this regard, nanofillers or polymers are treated or functionalized with modifiers or a compatibilizer is used to enhance the compatibility between the polymer matrix and nanoparticles. These techniques commonly provide a high interfacial interaction/adhesion between matrix and nanofiller which improve the final properties of nanocomposites. The significant interfacial interaction/adhesion leads to formation a third phase in polymer nanocomposites as interphase. Many experts have associated the large improvement of mechanical properties in the polymer nanocomposites to establishment of a strong interphase between polymer matrix and nanoparticles [15–19]. The role of interphase properties in the final performance of many nanocomposites such as nanocomposites from recycled polymers and shape memory polymer nanocomposites have been investigated [20,21].

The interfacial interaction/adhesion or the interphase level is a complicated subject which cannot be estimated by simple techniques. However, the theoretical studies can provide a large amount of valuable information for interphase and interfacial interaction in polymer nanocomposites. Our group has studied the properties of interphase in polymer nanocomposites by simple models for mechanical properties [15,18]. In these studies, many models such as Ji and Pukanszky were used to measure the thickness, modulus and strength of interphase.

Some researchers also have considered the interphase as a multi-layered phase, in which each layer has different properties. The characteristics of interphase layers were theoretically measured in different studies and the influences of the layer properties on the nanocomposite behavior were discussed [22–25]. Boutaleb et al. [23] assumed the thickness of interphase as a characteristic length scale and assessed the key role of the interphase on stiffness and yield stress of polymer nanocomposites. They compared the theoretical results with the experimental data in polymer/SiO_2 nanocomposites and reported some attractive results.

In the present paper, the tensile strength of interphase layers (σ_k) is modeled by several equations as different functions of the properties of polymer matrix and nanoparticles. The most suitable equation is chosen using the calculated interphase strength (σ_i) by the developed Leidner-Woodhams, Ji and Pukanszky models. The "σ_k" at the middle layer of the interphase is considered as average "σ_i" and compared with the calculations of micromechanical models to choose the best equation. The calculations are carried out for several samples from literature and the effects of the main parameters on "σ_i" are evaluated.

2. Background

The tensile strength of the interphase can be predicted by the model proposed by Leidner and Woodhams [26] for composites containing spherical particles as:

$$\sigma_c = (\sigma_i + 0.83\tau_m)\phi_f + \sigma_i S\phi_m \quad (1)$$

where "σ_c" and "σ_i" are the tensile strength of composite and interphase, respectively. Also, "ϕ_f" and "ϕ_m" are volume fractions of nanofiller and matrix, respectively. "τ_m" is the shear strength of matrix and "S" is a stress concentration parameter.

In our previous paper [15], the Leidner-Woodhams model was developed for polymer nanocomposites as:

$$\sigma_c = \left(\sigma_i + 0.83\frac{\sigma_m}{\sqrt{3}}\right)\phi_f - \sigma_i\frac{1}{B}\phi_m + \sigma_i\frac{1}{B} + \sigma_m \quad (2)$$

where "B" is the interfacial parameter in Pukanszky model [27] as:

$$\sigma_R = \frac{1-\phi_f}{1+2.5\phi_f}\exp(B\phi_f) \quad (3)$$

where "σ_R" is the relative tensile strength as σ_c/σ_m. "B" shows the level of stress transfer between matrix and nanofiller which is expressed as:

$$B = (1 + A_c\rho_f t)\ln\left(\frac{\sigma_i}{\sigma_m}\right) \quad (4)$$

where "A_c" and "ρ_f" are the specific surface area and density of nanofiller, respectively. Also, "t" is the thickness of interphase.

By rearranging of Eq. (2), "σ_i" is expressed as a function of "ϕ_f" as:

$$\sigma_i = \frac{\sigma_c - \sigma_m - 0.83\frac{\sigma_m}{\sqrt{3}}\phi_f}{(1+\frac{1}{B})\phi_f} \quad (5)$$

The average "σ_i" can be calculated by the latter equation for nanocomposites reinforced with spherical nanoparticles.

Ji et al. [28] developed the Takayanagi model and proposed a three-phase model for Young's modulus of nanocomposites taking into account the matrix, nanofiller and interphase. The Ji model for nanocomposites containing layered filler is given by:

$$E_c = E_m\left[(1-\alpha) + \frac{\alpha-\beta}{(1-\alpha)+\frac{\alpha(m-1)}{\ln(m)}} + \frac{\beta}{(1-\alpha)+\frac{(\alpha-\beta)(m+1)}{2}+\beta\frac{E_p}{E_m}}\right]^{-1} \quad (6)$$

$$\alpha = \sqrt{\left(2\frac{t}{d}+1\right)\phi_f} \quad (7)$$

$$\beta = \sqrt{\phi_f} \quad (8)$$

$$m = \frac{E_i}{E_m} \quad (9)$$

where "E_c", "E_m", "E_p" and "E_i" are Young's modulus of nanocomposite, matrix, filler and interphase, respectively. "d" is also the thickness or diameter of nanoparticles.

The average "t" for polymer/clay nanocomposites can be calculated by Ji model and the "σ_i" is obtained by applying the "t" value in Eq. (4). The detailed procedure for calculation of "σ_i" was explained in [29].

The thermo-mechanical properties of interphase between polymer matrix and nanoparticles change from nanoparticles properties to those of the polymer matrix. The interphase can be divided into n layers (Fig. 1) in which each layer has different properties from others.

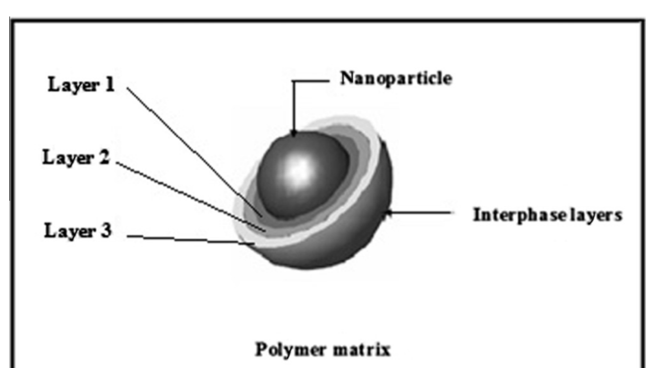

Fig. 1. Schematic illustration of interphase layers around a spherical nanoparticle in polymer nanocomposites (a 3-layered interphase).