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Research paper

Efficiency of stress transfer between polymer matrix and nanoplatelets in clay/polymer nanocomposites

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ABSTRACT

The Hui-Shia model, which considers the complete stress transfer between polymer matrix and particles (perfect interfacial adhesion), overpredicts the Young's modulus of clay/polymer nanocomposites (CPN). In this work, the effective aspect ratio and volume fraction of nanoclay are expressed assuming the imperfect load transfer, the minimum length of platelets required for efficient stress transfer (L_c) and the interfacial shear strength (τ). Additionally, "I" parameter as the level of stress transfer in CPN is defined and determined using the effective parameters. The large nanoclay platelets with low "L_c" give a high level of "I". Also, high "L_c" and slight "τ" observe the poor levels of effective parameters and Young's modulus of CPN. The "I" values are calculated for some samples which indicate the different levels of stress transfer in CPN. It is possible to analyze the levels of interfacial properties and stress transfer in CPN using the developed model.

1. Introduction

Polymer nanocomposites containing silicate layers (nanoclay) show high mechanical, physical, thermal and barrier properties by less content of nanofiller ($<$ 5 wt%) compared to micro-filler concentration in conventional composites (Ghari and Jalali-Arani, 2016; Monfared and Jalali-Arani, 2015; Norouzi et al., 2015; Olad et al., 2016; Shokri et al., 2016; Silva et al., 2016). The inorganic nanoparticles have a much higher modulus than polymer matrices which act as a strong reinforcement. Also, the molecular dimensions of nanoparticles have led to the development of many unexpected properties in polymer nanocomposites (Chaykar et al., 2016; Fasihi et al., 2013). The sheet-like platelets of nanoclay with very thin thickness (about 1 nm) and large length cause very large interfacial area and significant involvement between polymer and inclusion which change the overall properties of polymers such as stiffness, strength, crystallinity and chain conformation (Dehkordi et al., 2015; Shabanian et al., 2015; Tayefi et al., 2017). For these reasons, clay/polymer nanocomposites (CPN) have attracted much interest in academia and industries to suggest novel advanced materials for new applications or replace the old materials such as metals, plastics, composites and wood. The thermal stability, oxygen barrier property and biodegradability of albumin improved by addition of nanoclay (Dash et al., 2012). Also, nanoclay increased the mechanical properties and flame retardancy of poly (methyl methacrylate) (PMMA) (Patra et al., 2012). Moreover, it was shown that the mechanical properties of un-compatibilized and compatibilized blend nanocomposites depend on the localization of clay and its migration to interface (Aghjeh et al., 2015).

The mechanical properties of CPN such as modulus and strength primarily depend on the stress transfer mechanism between polymer matrix and rigid nanoparticles in which the properties of interface/interphase play a dominant role (Zare, 2015, 2016a). During the loading process, the level of stress transfer between polymer matrix and nanoparticles determines the extents of mechanical properties, because the stress is transferred from weak polymer matrix to rigid nanoparticles (Jia et al., 2016). In the case of good interfacial adhesion, a high level of stress can be transferred to nanoparticles leading to significant mechanical performances. However, poor interfacial adhesion between polymer matrix and nanoparticles cannot tolerate high stress and fails. As a result, the properties of interfacial regions and the level of stress transfer mainly affect the mechanical properties of polymer nanocomposites and much attention should focus on the bonding between polymer matrix and reinforcements.

Some previous reports have studied the effects of interface/interphase condition on the modulus and strength of polymer nanocomposites. Pukanszky (1990) and Ji et al. (2002) suggested several simple models which can calculate the interface/interphase properties in different polymer nanocomposites by experimental data of yield

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strength and Young's modulus, respectively. Also, many models were suggested or developed to correlate the modulus and strength of polymer nanocomposites to interphase properties such as thickness, modulus and strength (Shokrieh and Rafiee, 2010; Zare, 2016b,c). They clearly show that the interphase occupies a considerable volume of polymer nanocomposites and its properties significantly change the mechanical properties.

Hui and Shia (1998) suggested simple equations for Young's modulus of composites with aligned platelets assuming the perfectly bonded interface, i.e. complete stress transfer from polymer matrix to nanoparticles. However, the predictions of Hui-Shia model often do not match the experimental values, as mentioned in our previous work (Zare, 2016d). This occurrence is not unforeseen, since these equations are suggested based on a complete stress transfer from polymer to nanoparticles. The interfacial properties in nanocomposites are mainly weakened due to the poor compatibility between constituents and poor dispersion or aggregation/agglomeration of nanoparticles, which limit the interfacial surface area (Zare, 2016e,f). The low levels of interfacial/interphase properties in nanocomposites significantly reduce the mechanical properties. Shia et al. (1998) later assumed some effective parameters in the case of imperfect interfacial bonding in CPN which are explained and developed in this study.

Our previous work investigated the effects of incomplete interfacial adhesion on the modulus of CPN by Halpin-Tsai and Hui-Shia models by minimum length of platelets necessary for efficient stress transfer from matrix to clay (L_c) and interfacial shear strength (τ) (Zare, 2016d). "L_c" and "τ" were calculated for some samples using experimental modulus. Also, the effects of some parameters on the predicted modulus by these models were determined. In the present work, we focus on Hui-Shia model, which considers the complete stress transferring in nanocomposites and overpredicts the modulus. In other words, the Hui-Shia model is developed assuming the imperfect stress transfer in CPN. The effective aspect ratio and volume fraction of nanoclay are developed for whole length of platelets. Also, "I" parameter as the level of stress transfer in CPN is defined and determined by the effective parameters. Additionally, the effects of main variables such as clay length and aspect ratio, "L_c" and "τ" on the effective aspect ratio and filler fraction, "I" parameter and the predicted modulus are determined.

2. Hui-Shia model

The Hui-Shia model (Hui and Shia, 1998) was firstly suggested for Young's modulus of composites including unidirectional aligned platelets with perfect interfacial bonding between polymer matrix and platelet. According to this model, the longitudinal (E_{11}) and transverse (E_{22}) moduli are expressed as:

$$\frac{E_{11}}{E_m} = \frac{1}{1 - \frac{\varphi_f}{A}} \tag{1}$$

$$\frac{E_{22}}{E_m} = \frac{1}{1 - \frac{\varphi_f}{4}\left(\frac{1}{A} + \frac{3}{A+B}\right)} \tag{2}$$

$$A = \varphi_f + \frac{E_m}{E_f - E_m} + 3(1 - \varphi_f)\left[\frac{(1-g)\alpha^2 - \frac{g}{2}}{\alpha^2 - 1}\right] \tag{3}$$

$$B = (1 - \varphi_f)\left[\frac{3(\alpha^2 + 0.25)g - 2\alpha^2}{\alpha^2 - 1}\right] \tag{4}$$

$$g = \frac{\pi}{2}\alpha \tag{5}$$

where "E_m" and "E_f" are the Young's moduli of matrix and filler, respectively. "φ_f" is filler volume fraction and "α" is inverse aspect ratio of platelets as t/l, "t" and "l" are the thickness and length of disc-like platelets.

The modulus is a contribution of longitudinal and transverse moduli for a CPN containing completely 3D random dispersion of nanoclay in all directions. The Young's modulus of CPN in this condition (Fornes and Paul, 2003) is calculated by:

$$E_R = 0.49\frac{E_{11}}{E_m} + 0.51\frac{E_{22}}{E_m} \tag{6}$$

where $E_R = E_c/E_m$ and "E_c" is Young's modulus of nanocomposite.

Since many nanocomposites do not include the perfect interfacial adhesion between their components, Shia et al. (1998) assumed the incomplete stress transfer or imperfect bonding at polymer-filler interface and suggested the effective parameters for calculation of modulus. An imperfect interface cannot bear the large interfacial shear stress that develops during the applied strain that typically causes yielding or debonding at or near the interface region. Such deformation reduces the interfacial shear stress which introduces a slower build-up of normal stress in platelets. In this condition, a larger distance is required for the normal stress to reach the tensile strength of platelets (σ_f). As a result, a higher portion of platelet length is not fully loaded which decreases the reinforcing efficiency of nano-platelets.

A simple interface model was suggested by Shia et al. (1998) to designate the effect of imperfect load transfer on the reinforcing efficiency of platelets. The interfacial shear strength (τ) was assumed to be constant and nonzero over the imperfect interface. Fig. 1a illustrates the profiles of normal stress (σ) in a platelet at two possible cases. In the first case ($L_c \le x \le d/2$), "σ" reaches "σ_f" before the whole length of platelet debond. So:

$$\sigma = \sigma_f \tag{7}$$

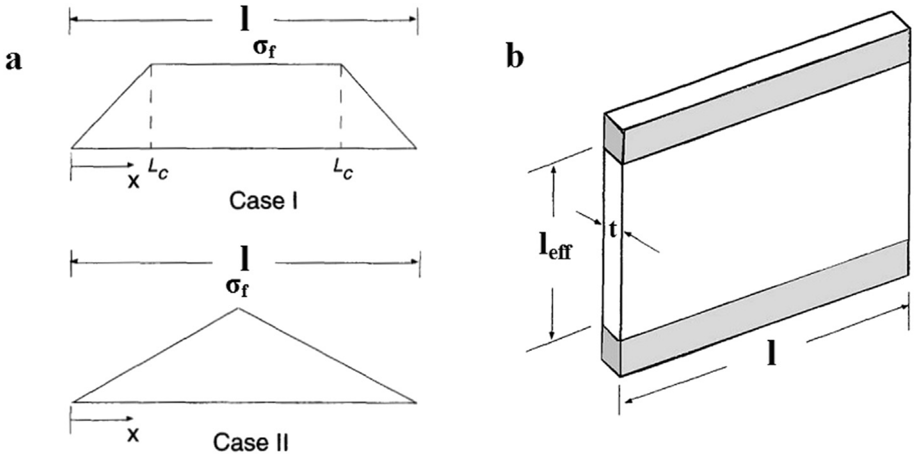

Fig. 1. a) The profiles of normal stress in platelets assuming imperfect stress transfer at two different states and b) illustration of "l_{eff}" due to deficient stress transfer.