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Predictions of Young's Modulus of Inorganic Fibrous Particulate-Reinforced Polymer Composites

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ABSTRACT: In this study, the factors affecting the Young's modulus of inorganic fibrous particulate-reinforced polymer composites were analyzed, and a new expression of the Young's modulus was derived and was based on a simplified mechanical model. This equation was used to estimate the composite Young's modulus. The estimated relative Young's modulus increased nonlinearly with increasing filler volume fraction. Finally, we verified the equation preliminarily by quoting the measured Young's modulus values of poly(butylene terephthalate)/wollastonite, polypropylene/wollastonite, and nylon 6/wollastonite composites reported in the literature. Good agreement was shown between the predictions and the experimental data of the relative Young's modulus values for these three composite systems. © 2013 Wiley Periodicals, Inc. J. Appl. Polym. Sci. 130: 2957–2961, 2013

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INTRODUCTION

The creation of inorganic fibrous particulate reinforced polymer composites is one of the major modification methods for polymer materials. The mechanical properties and reinforcing and toughening mechanisms for the fibrous particulate-reinforced polymer composites have been extensively studied over the past 2 decades.[1–5] These fibrous particles include wollastonite,[1–3] tremolite,[4] and asbestos.[5] Liu et al.[4] investigated the effect of a silane coupling agent on the mechanical and thermal properties and morphology of tremolite/PA1010 composites; they found that the tensile strength and notched Izod impact strength of the modified tremolite composites were improved simultaneously compared to those with pure tremolite. Xu et al.[5] measured the performance of fiber-reinforced asphalt concrete under environmental temperature and water effects; the results show that the fibers significantly improved the asphalt concrete rutting resistance, fatigue life, and toughness. Also, the split in the indirect tensile strength at low temperatures was also improved.

Young's modulus is an important utilization properties of solid materials. For polymer composites, the factors affecting Young's modulus are complicated and include the nature of the matrix resin and filler, compatibility between them, materials processing technology and conditions, dispersion or distribution of the filler in the matrix, and interfacial structure and morphology.[6,7] There have been several quantitative descriptions for the Young's modulus of inorganic particulate filled polymer composites, and the famous equation among them is the Young's modulus equation, which is based on the mixture role.[8] More recently, Liang[9,10] studied the reinforcing mechanisms of short inorganic fiber filled polymer composites and derived a new Young's modulus equation and a new tensile strength equation.

The objectives in this study were to investigate the major factors affecting the Young's modulus of inorganic fibrous particulate-reinforced polymer composites to propose a new quantitative description of Young's modulus for this kind of polymer composite.

BASIC EQUATION

Mechanical Model

The basic hypotheses of theoretical analysis used in this study were as follows: (1) the inorganic fiber is a roughly square column body, (2) the dispersion of the inorganic fibrous particles in the matrix is uniform, (3) the relationship between the stress and strain follows Hooke's law, and (4) the fillers in the resin matrix are oriented completely along the force direction. Accordingly, we took the matrix resin as a small rectangular parallelepiped with only an inorganic fibrous particle in its center, as shown in Figure 1.

Mathematical Model

According to the mechanical model shown in Figure 1 and from Hooke's law, assumption 3, and the principle of force balance, we have

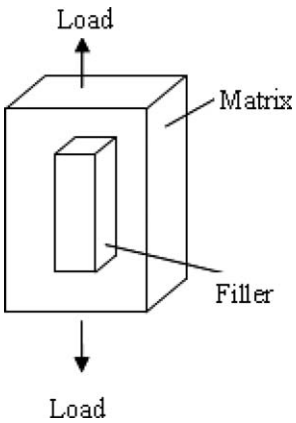

Figure 1. Element mechanical model of the polymer/fibrous particle composites.

$$\sigma \cdot S = \sigma_m \cdot S_m + \sigma_I \cdot S_f \tag{1}$$

where σ is the normal stress upon cross section of the cube, S is the cross-sectional area of the cube, S_m is the effective cross-sectional area of this cube, S_f is the fibrous particle cross-sectional area, σ_m is the normal stress upon the effective cross section of the cube, and σ_I is the normal stress upon cross section of the interface between the matrix and the fibrous particle.

S_m can be determined from the relationship between the cube size and volume fraction. The deformation of both the filler and the body is very small within the elastic limit; thus, one might consider their strains to be approximately equal to each other. That is

$$\varepsilon_c \approx \varepsilon_m \approx \varepsilon_f \tag{2}$$

where ε_c, ε_m, and ε_f are the elastic strains of the composites, continuous phase resin, and inorganic fibrous particles, respectively.

According to the definition of Young's modulus and the filler volume fraction (&phis;$_f$) and with the introduction of the concept of interfacial layer stiffness, we derived a Young's modulus equation from eqs. (1) and (2) as follows:

$$E_c = E_m\left[1 + (\lambda - 1)\phi_f^{2/3}\right] \tag{3}$$

$$\lambda = E_I / E_m \tag{4}$$

where λ is the interfacial interaction parameter of the polymer composites and E_c, E_m, and E_I are the Young's moduli of the composites, matrix resin, and interface between the filler and matrix, respectively.

If we define the relative Young's modulus (E_R) as follows:

$$E_R = E_c / E_m \tag{5}$$

Equation (3) may be rewritten as follows:

$$E_R = 1 + (\lambda - 1)\phi_f^{2/3} \tag{6}$$

In general, the value of λ may be determined roughly from the experimental data.

ANALYSIS AND COMPARISON

Analysis

Equations (3) and (6) describe the relationship between the Young's modulus of inorganic fibrous particulate reinforced polymer composites and the Young's moduli of the resin matrix and filler, the filler volume fraction, and λ. λ presents the interfacial interaction between the filler and the matrix; it is related to the properties of the filler and matrix, such as their stiffness and the crystallization properties in the interlayer. Substituting various values of the filler volume fraction and λ into eq. (6), one may estimate the corresponding relative Young's modulus for inorganic fibrous particulate reinforced polymer composites. Then, plotting the calculated relative Young's modulus against the filler volume fraction, one may obtain the relationship between the estimated relative Young's modulus and the filler volume fraction for the composites; the results are shown in Figure 2. With increasing the filler volume fraction, the estimated relative Young's modulus increases nonlinearly when λ is fixed. In addition, the sensitivity of the estimated relative Young's modulus to the filler volume fraction is enhanced with an increase in λ.

As stated previously, there are several expressions for predicting the inorganic particulate-reinforced polymer composites; among the equations characterizing the Young's modulus, the mingling rule[8] shown is the most simple and common to apply:

$$E_c = E_m\left(1 - \phi_f\right) + E_f\phi_f \tag{7}$$

where E_f is the Young's modulus of the filler.

In many cases, it is just an approximation to estimate the Young's moduli of polymer composites by the mingling rule, especially in the case of low filler concentration because the mingling rule does not consider the interfacial states between the filler and matrix or the particle shape, size and size distribution, dispersion of particles in the matrix, and so on.

For flaky particulate-reinforced polymer composite systems, the Halpin–Tsai equation is considered to be a suitable equation for predicting the Young's moduli for polymer composites:[11]

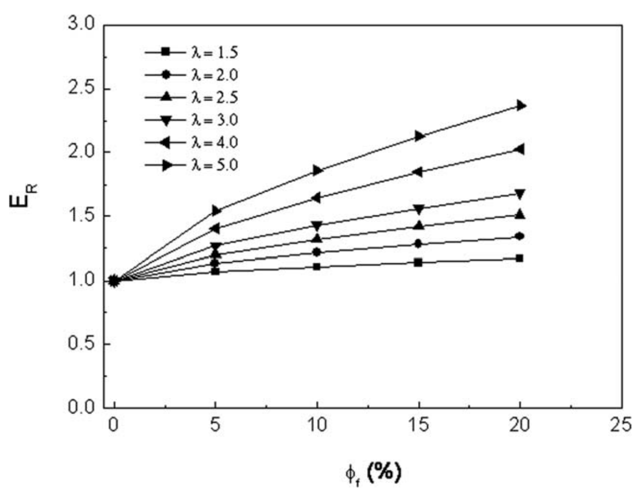

Figure 2. Relationship between the estimated Young's modulus and filler volume fraction of the inorganic fibrous particulate-reinforced polymer composites.

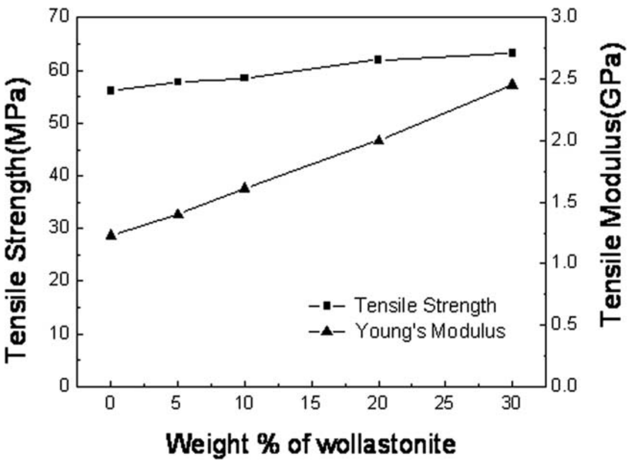

Figure 3. Tensile strength and tensile modulus of the PBT/wollastonite composites.[1]

$$E_c = E_m\left(\frac{1+I\eta\phi_f}{1-\eta\phi_f}\right) \tag{8}$$

$$\eta = \frac{m-1}{m+I} \tag{9}$$

where η is a parameter, m is equal to E_f/E_m and I is a parameter related to the filler shape and is defined as follows:

$$I = 2\zeta \tag{10}$$

where ζ is the particle aspect ratio.

Through a comparison of eqs. (7) and (8), one find that more filler parameters, including the modulus and particle aspect ratio, need to be known before these two equations can be used to estimate the Young's moduli of inorganic fibrous particulate-reinforced polymer composites.

Comparison between the Predictions and Measured Data

Poly(butylene terephthalate) (PBT)/Wollastonite Composites. Deshmukh et al.[1] evaluated the mechanical and thermal properties of PBT composites reinforced with wollastonite; their tensile strength and Young's modulus exhibited a marginal increase, as shown in Figure 3. Here, the density of PBT was 1.3 g/cm^3, the density of wollastonite was 2.9 g/cm^3, and the average particle size was 30 μm. Young's modulus of the PBT/wollastonite composites increased nonlinearly with increasing filler weight fraction. Moreover, as shown in Figure 3, the Young's modulus of PBT was about 1.23 GPa, and λ was about 4.

Substituting the previous data into eq. (6), we estimated the values of the relative Young's modulus of the PBT/wollastonite composites. Then, plotting the estimations and the experimentally measured data of the relative Young's modulus again the filler volume fraction, we made a comparison between the estimations and the experimentally measured data of the relative Young's modulus for the PBT/wollastonite composites, as shown in Figure 4. Here, the correlation between the weight fraction and volume fraction for the filler could be expressed as follows:[12]

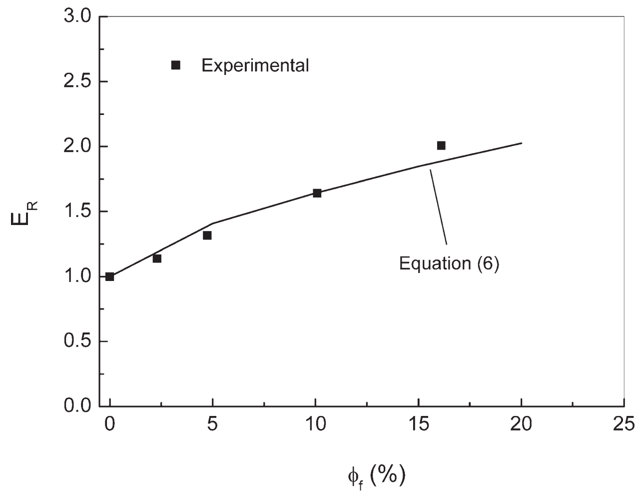

Figure 4. Comparison between the estimations and experimental data of Young's modulus for the PBT/wollastonite composites.

$$\phi_f = \frac{W_f}{W_f(1-\chi)+\chi} \tag{11}$$

$$\chi = \frac{\rho_f}{\rho_m} \tag{12}$$

where ρ_f and ρ_m are the densities of the filler and matrix, respectively, ϕ_f is the filler volume fraction, and W_f is the filler weight fraction.

The predictions of the relative Young's modulus for the PBT/wollastonite composites were roughly close to the experimentally measured data shown in Figure 3.

Nylon 6/Wollastonite Composites. Unal et al.[2] studied the mechanical properties and morphology of nylon 6 hybrid composites; the fillers included glass beads, kaolin, talc, and wollastonite. They found that the tensile strength of the nylon 6/wollastonite composite was higher than that of the neat resin, and the Young's modulus increased with increasing weight fraction of wollastonite, as shown in Figure 5. Here, the density of nylon 6 was 1.14 g/cm^3; the density and average particle size of wollastonite were 2.9 g/cm^3 and 46.8 μm, respectively. In

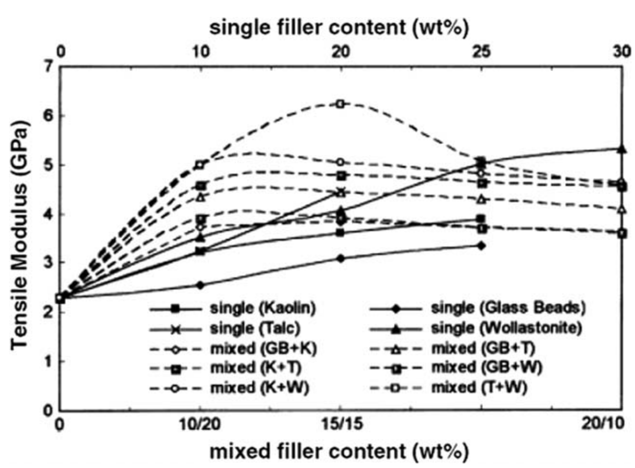

Figure 5. Tensile modulus–filler weight fraction curves for the nylon 6 composites.[2] GB = glass bead, K = kaolin, T = talc, W = wollastonite.

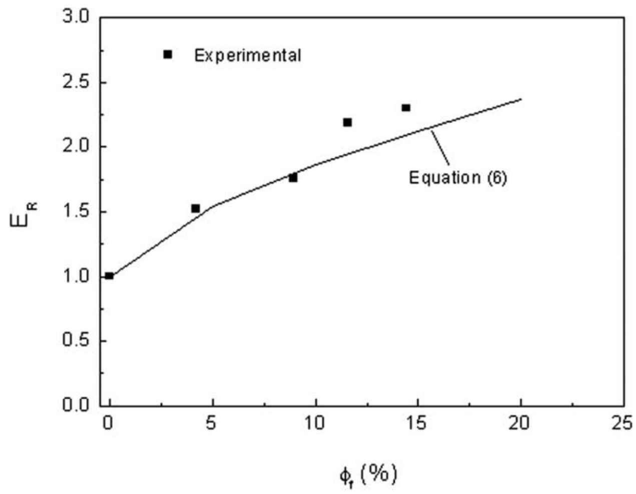

Figure 6. Comparison between the estimations and experimental data of Young's modulus for the nylon 6/wollastonite composites.

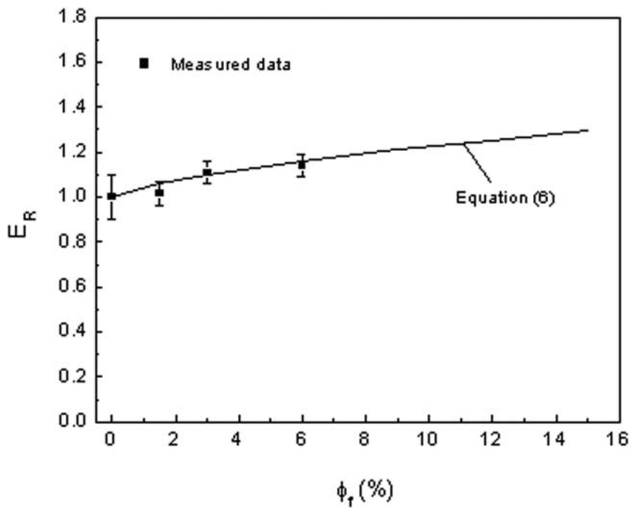

Figure 7. Comparison between the estimations and experimental data of Young's modulus for the PP/wollastonite composites.

addition, the particle aspect ratio was 10:1. As shown in Figure 5, Young's modulus of the nylon 6 was about 2.31 GPa, and the λ value was about 5.

Substituting the previous data of the nylon 6 and wollastonite into eq. (6), we estimated the values of the relative Young's modulus of the nylon 6/wollastonite composites. Then, plotting the estimations and experimentally measured data of the relative Young's modulus against the filler volume fraction, we made a comparison between the estimations and the experimentally measured data of the relative Young's modulus for the nylon 6/wollastonite composites, as shown in Figure 6.

As shown, the predictions of the relative Young's modulus for the nylon 6/wollastonite composites were roughly close to the experimentally measured data shown in Figure 5.

Polypropylene (PP)/Wollastonite Composites. Luyt et al.[3] investigated the morphology and mechanical and thermal properties of composites of PP and nanostructured wollastonite filler; the results show that Young's modulus slightly increased with wollastonite loading, as shown in Table I. Here, σ is the standard deviation, σ_b is the tensile strength at break, and ε_b is the tensile elongation at break.

According to the experimental data reported in ref. 6, the Young's modulus of PP was 0.65 GPa, and λ was about 1.5.

Table I. Mechanical Properties of the Pure PP and PP/Wollastonite Nanocomposites[3]

Filler content (vol %)	$E_c \pm \sigma$ (GPa)	$\sigma_b \pm \sigma$ (MPa)	$\varepsilon_b \pm \sigma$ (%)
0	0.65 ± 0.2	19.8 ± 0.2	23 ± 4
1.5	0.66 ± 0.1	20.4 ± 0.3	7 ± 2
3	0.72 ± 0.1	19.6 ± 0.3	6 ± 2
6	0.74 ± 0.1	18.6 ± 0.4	5 ± 1

Substituting these data into eq. (6), we estimated the Young's modulus of the PP/wollastonite composites. Then, plotting the predicted and measured Young's moduli of the PP/wollastonite composites against the filler volume fraction, we found the results that are shown in Figure 7. Similarly, good agreement was shown between the estimations of the relative Young's modulus and the measured data for the PP/wollastonite composites, as shown in Table I.

CONCLUSIONS

Equation (6) describes the correlation between the relative Young's modulus for inorganic fibrous particulate reinforced polymer composites and the filler volume fraction as well as λ. It should be convenient to use because of its simplicity and because the parameters in it are easily determined. The estimated relative Young's modulus of the inorganic fibrous particulate reinforced polymer composites increased nonlinearly with increasing filler volume fraction, and the sensitivity of the relative Young's modulus to the filler volume fraction increased with increasing λ.

The relative Young's moduli for the three composite systems, the PBT/wollastonite, nylon 6/wollastonite, and PP/wollastonite composites, were estimated with this equation. Good agreement was found between the predictions and the experimental data of the relative Young's moduli reported in literature.

REFERENCES

1. Deshmukh, G. S.; Peshwe, D. R.; Pathak, S. U.; Ekhe J. D. *Trans. Indian Inst. Met.* **2011**, *64*, 127.
2. Unal, H.; Mimaroglu, A.; Alkan, M. *Polym. Int.* **2004**, *53*, 56.
3. Luyt, A. S.; Dramićanin, M. D.; Antić, Ž.; Djoković, V. *Polym. Test* **2009**, *28*, 348.

4. Liu, X. L.; Han, Y.; Gao, G.; Li, Z. Y.; Liu, F. Q. *Chin. J. Polym. Sci.* **2008**, *26*, 255.

5. Xu, Q. W.; Chen, H. X.; Prozzi, J. A. *Const. Build Mater.* **2010**, *24*, 2003.

6. Liang, J. Z.; Li, R. K. Y. *Polym. Compos.* **1998**, *19*, 698.

7. Liang, J. Z.; Li, R. K. Y.; Tjong, S. C. *Polym. Compos.* **1999**, *20*, 413.

8. Liang, J. Z. Reinforcing and Toughening Theory of Polymer Composites; South China University Press: Guangzhou, **2012**.

9. Liang J. Z. *Polym. Test.* **2011**, *30*, 749.

10. Liang J. Z. *Compos. B* **2012**, *43*, 1763.

11. Halpin, J. C.; Kardos, J. L. *Polym. Eng. Sci.* **1976**, *16*, 344.

12. Liang, J. Z.; Li, R. K. Y. *J. Reinf. Plast. Compos.* **2001**, *20*, 630.