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ORIGINAL PAPER

Prediction of tensile modulus of nanocomposites based on polymeric blends

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Abstract A simple model was proposed for predicting the Young's modulus of nanocomposites based on polymeric blends. First, a simple model was derived for binary blends containing only two polymers. This model is more useful for those blends with high degree of continuity. Therefore, the morphology of the blend is divided into parallel and series regions and the percolation theory is used to calculate the volume fraction of these phases. In the next step, the addition of nanoclay, as a third component, is being considered. These nanoparticles may possibly find locations at the matrix, minor or interface. In the latter case, the model was expanded into a three-phase model including the matrix, dispersed and a third phase containing nanoclay which itself was split into series and parallel sections. A model related to the reinforcing effect of nanoclay was employed and combined with the above model to estimate the modulus of this ternary nanocomposite. The experimental data which is obtained from nanocomposite based on low-density polyethylene/thermoplastic starch/Cloisite 30B were compared with the model results and revealed a good agreement with each other. Also, the model predictions were compared with other experimental data from literature sources to verify the model accuracy. The comparison showed that the model predictions can predict the experimental data rationally. This model can be used to determine the structure of a nanocomposite without any other expensive tests.

Keywords Nanocomposites · Polymer blends and alloys · Mechanical properties · Tensile modulus modeling · Continuity

Abbreviations

Φ_1, Φ_2, Φ_3	Volume fraction of matrix, minor and the third phase, respectively
Φ_{cr}	Percolation threshold
Φ_0	Prefactor volume fraction
v_1,v_2,v_3	Corrected volume fraction of matrix, minor and the third phase, respectively
Φ_n	Nanoclay volume fraction of nanoclay
v_f	Corrected nanoclay volume fraction
S, p	Series and parallel phases, respectively
E_i	The modulus of phase ith
I_s, I_p	The thickness of series and parallel of the third phase, respectively
t	Plate thickness of nanoclay
τ	Interface
k	One of the model parameters
γ_i, γ_i^d, γ_i^p	Surface tension, dispersive component and polar component of phase i, respectively
γ_{ij}	Interfacial tension between i and j phases
ω_{12}	The wettability parameter

Introduction

Modeling the mechanical properties of polymer blends and nanocomposites is an interesting area in polymer science and exciting method for the design of high performance materials. There are many models for predicting the modulus of polymer blends as a function of the composition. The simplest models are rule of mixtures and inverse

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