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ORIGINAL PAPER

Modeling of blend-based polymer nanocomposites using a knotted approximation of Young's modulus

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Abstract A "knotted approximation" (KA) is proposed in order to predict the Young's modulus of blend-based polymer nanocomposites (BPNs). The BPN system is considered to have two fundamental constituents, a binary polymer blend and an effective phase (nanoparticle-containing phase). Therefore, the KA model was designed to combine the results of two different models which govern different hypothetical constituent elements of BPN systems. This was very helpful to enhance the accuracy of KA model by controlling parameters which affect each model. Furthermore, the application of different models was investigated to obtain the most efficient mathematical framework. Despite simple methodology of the KA model, the consistency of governing models on each constituent was considered as an important factor. Based on the wetting coefficient, the nanoparticles were considered to be in an individual phase of the binary polymer blend, so it could satisfy the presumptions of the effective phase. Considering the strong influences of nanoparticles on the percolation threshold of polymer phases, a general method was proposed to consider this important phenomenon. As a result, combining the fundamental concepts of KA constituent models enabled it to involve a wide range of critical parameters related to the BPN systems, e.g., morphology, random orientation of nanoparticles, nanoparticle/polymer interphase, phase inversion, polymer phase percolation threshold, etc. To evaluate the accuracy of KA model, different samples of polyamide/polyolefin elastomer/Cloisite 30B were prepared and subjected to stress–strain test in order to compare the predicted and actual values of BPNs Young's modulus.

Keywords Nanocomposite · Young's modulus · Modeling · Knotted approximation

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Introduction

Polymer nanocomposites as well as polymer blends are of the most attractive materials in the polymer family due to their high performance and ease of production [1, 2]. There have been many investigations carried out in order to come up with new and unique ways to produce these materials, while some other investigations have focused on the study of their specific mechanical properties [2]. Modeling, which is defined as an easy way to simulate the systematic reactions against environmental phenomena, is always considered as an engineering way to overcome the experimental obstacles to obtain final values of mechanical properties, e.g., modulus, tensile strength, impact strength, etc. [3]. So far, many models have been proposed by which the modulus of a nanocomposite or polymer blend can be predicted. On the other hand, it is quite interesting to investigate the mechanical properties of the combination of these two polymer groups, while they are both meant to enhance some physical and mechanical properties of an individual polymer phase [4]. Blend-based polymer nanocomposites (BPNs) are considered as a new generation of materials in which the mechanical and physical properties of a polymer blend are widely improved [5–7]. Two dispersed phases should be considered separately in a BPN system, which are nanoparticles and polymer-dispersed