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Estimation of effective elastic properties of polymer/clay nanocomposites: a parametric study

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Abstract

In this work, a 3D finite element model has been developed to compute the macroscopic elastic properties of polymer/clay nanocomposites (PCNs) from the microstructure morphologies and the elastic behaviour of each phase. Microstructural parameters of clay or clay stacks such as elastic properties, aspect ratio, interlayer spacing and clay volume fraction have been taken into account in the proposed models. A parametric study of the effect of these parameters on the macroscopic elastic properties of PCNs has been carefully investigated. The results show that the macroscopic rigidity of PCNs materials depends not only on the clay volume fraction but also on the dispersion state of clay platelets in the polymer matrix. An exfoliated structure may improve the macroscopic rigidity of PCNs much more efficiently than intercalated ones, particularly at high volume fraction of clays. The key role of interphase on the mechanical properties enhancement of PCNs has also been demonstrated. In addition, the partially exfoliated morphology, in which individual clay layers and intercalated blocks are simultaneously present in the polymer matrix, has been studied. The last morphology is commonly encountered in PCN processing, especially when high clay content is used. The comparison with the experimental and theoretical results extracted from the literature has been performed.

Keywords: effective elastic properties, clay, polymer, exfoliated, intercalated, partially exfoliated, interphase

1. Introduction

In the last decade, polymer/clay nanocomposites (PCNs) have attracted considerable attention in academic and industry due to their superior properties such as rigidity, thermal stability and flame retardant, gas barrier far from those of conventional microcomposites. In addition, these improvements are obtained without loss of optical clarity and recycling while keeping the light weight of polymeric materials [1, 2, 3].

Depending on several factors including the nature of constitutive components (silicate layer, surfactant and polymer matrix) and the preparation method, the dispersion state of fillers such as pristine or modified clay in a polymer matrix may be quite different from

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