Composites Part B 89 (2016) 303–315

Contents lists available at ScienceDirect

Composites Part B

journal homepage: www.elsevier.com/locate/compositesb

On the tensile behavior of clay–epoxy nanocomposite considering interphase debonding damage via mixed-mode cohesive zone material

Reza Maleki Moghadam*, Saeed Saber-Samandari**, Seyyed Ahmad Hosseini

New Technologies Research Center, Amirkabir University of Technology, PO Box 1591633311, Tehran, Iran

ARTICLE INFO

Article history:
Received 13 April 2015
Received in revised form
10 August 2015
Accepted 20 November 2015
Available online 7 January 2016

Keywords:
A. Nano-structures
B. Debonding
B. Mechanical properties
C. Finite element analysis (FEA)

ABSTRACT

This paper proposes a constitutive 3D multi-scale four-phase model of exfoliated clay/epoxy nanocomposites. The model encompasses a clay platelet, non-perfect bond interactions, an interphase region and an encircling matrix. The outcomes divulge a pronounced influence of the cohesive zone material (CZM) on the tensile behavior of the models which is more significant in higher clay weight percentage. Moreover, the results demonstrate higher load transfer efficiency in the model possessing a CZM and debonding compared with a model without a CZM. The results are consistent with published experimental investigations, and the model can be used as a viable tool to scrutinize the behaviors of clay–polymer nanocomposites.

1. Introduction

The breakthrough of nano-reinforcements, including carbon nanotubes and nano-particles, has received great attention in recent research because of their extraordinary influence on augmenting polymer stiffness, strength, etc., in presence of small amount of reinforcements [1–8]. Among these, Clay imparts striking properties in which Montmorillonite have motivated much enthusiasm in both academic and industrial sectors because the addition of a small amount of nanoclay can substantially enhance the mechanical properties of pristine polymers [9–16]. Understanding the relation between nanostructure, nano-scale parameters and the overall behavior of nanocomposites is crucial in the development of such materials. Many experimental studies have been carried out on the mechanical behavior of clay-polymer nanocomposites [17–20]. The clay particle structure is either exfoliated or intercalated. For enhanced functional properties of nanocomposites at the same clay concentration the former is preferred [21]. An exfoliated polymer-clay nanocomposite (PCN) was developed by the Toyota group by synthesizing a nylon 6/clay nanocomposite [22,23]. Abdul Azeez et al. [24] reviewed the processing and properties of clay/epoxy nanocomposites with an emphasis on the influence of processing techniques, clay modifiers and curing agents on the mechanical properties of nanocomposites. Khanbabaei et al. [25] synthesized clay–epoxy nanocomposites and examined the effects of adding different contents of nanoclays on the physical, mechanical, and thermal properties of the epoxy resin system. Experimental and numerical investigations have been conducted by Silani et al. [26] to explain the effect of clay on the ductility reduction of the nanocomposite. Moreover, the results of the crack initiation simulated in dog-bone samples by extended finite element method (XFEM) were in good agreement with those from the experimental method. Katti et al. [27] have reported the nature of the interactions between clay and polymer and between clay and organo modifier in polymer–clay nanocomposites through experimental methods and molecular dynamics simulations. Augmenting epoxy toughness by the combination of both nanoclay and thermoplastic materials have been introduced by Rostamiyan et al. [28]. The results obtained indicated that the tensile, compressive and impact strength of the new ternary nanocomposites were ameliorated from those of the neat resin. Saber-Samandari et al. [29] studied the effect of processing variables on the mechanical properties of a clay/epoxy nanocomposite produced in a centrifuge with varying processing conditions such as centrifuge rotor speed and curing temperature. The results demonstrated that the elastic

---

* Corresponding author.
** Corresponding author.
E-mail addresses: reza.malekimoghadam@gmail.com (R. Maleki Moghadam), saeedss@aut.ac.ir (S. Saber-Samandari).

http://dx.doi.org/10.1016/j.compositesb.2015.11.043

modulus increased for clay content up to 6 wt% but the rate of modulus increase declined above 6 wt%. Shokrieh et al. [30] investigated the effects of adding nanoclay on the mechanical properties of an epoxy polymer. The results showed that the tensile and flexural moduli, compressive strength and the fracture toughness increased by 12.5%, 13.3%, 7.4% and 25.5%, respectively, with the addition of nanoclay content, while the tensile and flexural strengths as well as strain to failure decreased. From the modeling approaches point of view, extensive analytical and numerical methods have been developed with most devoted to finite element methods as viable tools to analyze nanostructures [31–35]. Most investigations have proposed a 2D finite element representative volume element to study the mechanical behavior of exfoliated and intercalated clay-nanocomposites [36–38]. An analytical homogenization method relying on different micromechanical models (i.e. Mori–Tanaka, self-consistent and Lielens's) with finite element modeling have been exploited by Pahlavanpour et al. [39] to illustrate the mechanical behavior of polymer–clay nanocomposites. The results show that the Mori–Tanaka was the most reliable micromechanical model for the simulated cases. Mohammadpour et al. [40] predicted the mechanical behavior of polypropylene composites doped with carbon nanotubes (CNT) using a CZM model to consider the interfacial shear stress between the CNT and the matrix. Pisano et al. [41] predicted the strength reduction for the intercalated epoxy/clay nanocomposites via finite element model considering gallery failure. The results indicated that gallery failure is a cause of nanocomposite strength reduction and depending on the morphology, interfacial debonding is as important as gallery failure in affecting the nanocomposite strength. The initiation and growth of micro-cracks in nanoclay reinforced polymer composites were analyzed numerically by Dai and Mishnaevsky Jr. [42] using 3D micromechanical unit cell models taking into account different crack growth criteria. Additionally, Song et al. [43] introduced a computational model for clay–epoxy nanocomposites comprising an epoxy matrix and a silicate layer to study their damage mechanism. From the results, it can be deduced that the damage of epoxy–clay nanocomposites could be caused by several factors such as the splitting of the gallery layer, debonding of the interphase layer or a stress concentration at the clay particle and matrix interface. In other literature, the self-consistent method has been used to attain the mechanical properties of polymer–clay nanocomposite materials [44,45]. Dong et al. [46] represented the overall nanocomposite behavior through a combination of real data of the micro/nanostructure utilizing transmission electron microscopy (TEM) and scanning electron microscope (SEM) and of the fundamental material characteristics of the constitutive phases. According to the above-mentioned literature, a detailed 3D multiphase model that is capable of capturing all length-scale parameters at the nano-micro scale is lacking. Hence, the present work proposes a capable 3D four-phase finite element model that can elucidate the debonding damage between clay and the interphase, the elasto-plastic behavior of the matrix and the effects of the interphase parameters on the mechanical behavior of the clay–polymer nanocomposite materials.

2. Constitutive finite element modeling of exfoliated clay–epoxy nanocomposites

High exfoliation is desirable for enhancing the functional properties of nanocomposites; however complete exfoliation is never achieved. In this work, the proposed FE model of a representative volume element (RVE) consisting of a clay platelet, the surrounding matrix and an interphase region considering interfacial debonding is established via the ANSYS 15 commercial package [47]. According to substantial material behavior on a macro scale, the load transfer occurs from the surrounding matrix to the clay platelets. Thus we adopt a short-clay model, entirely embedded in an epoxy matrix which hereinafter is called “Short RVE” to investigate the load transferring phenomena on the nano/micro scale. As conclusion, “long RVE” nanocomposites model, the homogenization method, excluding debonding damage and 2D FE modeling cannot substantially capture the tensile behavior and load transferring phenomena of clay–polymer nanocomposites. The aforementioned models are shown in Fig. 1.

A four-phase short RVE model including a clay platelet, an interphase region, clay–epoxy interactions and an encircling epoxy polymer that is capable of capturing interphase debonding, elastoplastic behavior of a polymer, load transferring phenomena and interphase parameters influences on the tensile behavior of clay–polymer nanocomposites is constructed. The modeling procedure of a RVE is depicted in Fig. 2.

2.1. Clay platelet

The clay platelet is simulated as an elastic isotropic material with the same material properties as Montmorillonite, a well-known clay platelet. The thickness of each platelet is assumed to be 1 nm [48,49]. The SOLID 186 element has been employed to construct the finite element of the clay model. This element possesses 20 nodes with three degrees of freedom per node which are transitional in x, y and z directions [47]. Additionally, because of the usage of an intermediate node on each edge of the element, it has higher order shape function and thus results in a higher accuracy.

2.2. Surrounding epoxy matrix

Considering various weight percentages of clay, the epoxy resin has been simulated with the SOLID 186 element. The constructed resin is treated as an isotropic material with elasto-plastic and failure properties capable of exhibiting plastic behavior in the matrix during tensile analysis. The multi-linear isotropic hardening plasticity is adopted to simulate a finite element model which may be preferred for cycling where the kinematic hardening could exaggerate the Bauchinger effect. Furthermore a maximum of 100 stress-strain points can be defined to explain polymer behavior [47]. Hence the stress-strain parameters and failure criteria of epoxy have been extracted from datasheets.

2.3. Interphase region and interactions of clay/epoxy

The key issue defining the efficiency of improving the properties of clay–polymer nanocomposites at micro-scale is the load transferring phenomenon from the resin to the clay platelet through the interphase-interactions between the clay and the matrix. Thus, accounting for the load transferring mechanism from the matrix to the clay, modeling the interphase region plays a crucial role in a proper understanding of the polymer clay nanocomposites (PCN). Consequently, the aforementioned region is broken down into two segments comprising the mobility region and the interactions between epoxy and clay which are simulated by the interphase and the CZM model, respectively, according to Fig. 2.

2.3.1. Interphase region

For both intercalated and exfoliated clay particles, the outer surface of the clay is in contact with the matrix which is defined as interphase in this region. The interphase region between the surrounding matrix and the clay can exhibit as a mobility region [50] for which the mechanical properties vary from the clay to the matrix with different values reported for the thickness magnitude