Composites Science and Technology 74 (2013) 67–77

Contents lists available at SciVerse ScienceDirect

Composites Science and Technology

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

Damage evolution in nanoclay-reinforced polymers: A three-dimensional computational study

Gaoming Dai *, Leon Mishnaevsky Jr. *

Department of Wind Energy, Technical University of Denmark, Risø Campus, Frederiksborgvej 399, DK-4000 Roskilde, Denmark

ARTICLE INFO

Article history:
Received 9 July 2012
Received in revised form 1 October 2012
Accepted 3 October 2012
Available online 13 October 2012

Keywords:
A. Nanoclay
A. Nanocomposites
C. Finite element analysis (FEA)
C. Modeling

ABSTRACT

Initiation and growth of microcracks in the nanoclay reinforced polymer composites were analyzed in numerical experiments using 3D micromechanical unit cell models. An original program code for the automatic generation of FE unit cells with multiple disk-shaped nanoplatelets, with high aspect ratio, clustered or exfoliated, randomly arranged or inclined, was developed. A four phase model of nanocomposites which includes the effective interface between the nanoplatelets and polymer, as well as interplatelet and outer phases, was used in the simulations. Different crack growth criteria were compared, including the 3D Benzeggagh and Kenane law (BK law) criterion, the 3D Wu and Reuter law (power law) criterion and the Reeder law criterion. The effects of the platelet aspect ratio, clustering and orientation effects on the crack propagation are studied in numerical experiments. It was observed that the increasing aspect ratio leads to the increasing Young modulus, but decreasing strength. The clustering of disks had an adverse effect, meaning increased strength and lower stiffness. In the simulations, damage mechanisms such as crack deflection and delamination were observed.

1. Introduction

Nanoclay-reinforced polymers are considered among most promising materials for energy, aerospace, marine and automotive applications. The possibilities of drastic enhancement of the mechanical properties and strength of polymers and composites by using nanoreinforcement attracted great interest of the research community [1–5]. The exact knowledge of the deformation and damage mechanisms in nanocomposites, effect of structural properties of nanoclay (e.g., shape, aspect ratio, etc.) and its morphologies (orientation, clustering, etc.) play an important role in evaluating and optimally exploiting the potential of nanoreinforcement for the improvement of material properties [6–12].

The purpose of this work is to develop computational models and methods which allow analyzing the damage mechanisms and mechanics of nanoclay-reinforced polymers under mechanical loading, using the virtual (computational) experiments. A 3D nanocomposites computational model, which includes the effective interface concept and is able to account for mixed mode crack initiation and propagation, is proposed. Physical parameters such as nanoplatelet aspect ratio, clustering and orientation that affect the damage performance of nanocomposites are studied systematically, and the recommendations toward to enhancement of the materials properties by varying the microstructures are developed.

2. Nanoclay-reinforced polymers: damage mechanisms

The modifications of materials structures and multiscale structure control represent promising possibilities for the optimal design of materials with enhanced properties [9–11]. In order to optimally realize the potential of nanoreinforcement in polymer composites, the exact knowledge of the nanoreinforcement effect of strength and damage of composites, and computational models describing these effects are necessary.

Damage mechanisms in nano-reinforced composites are described typically as the initiation of micro-cracks and their propagation along the matrix–clay interface and inside the matrix. Damage mechanism phenomena such as crack deflection, plastic deformation and crack pinning appear simultaneously. Besides, localized shear bands initiated by the stress concentrations surrounding the nano-particles, micro-cracks formation inside nanocomposites, delamination or debonding between nano-particles and matrix, the fracture surface area increment and matrix deformation are the major toughening mechanisms [12–21].

Typically, it is expected that introducing nano-particles in the polymer matrix should lead to the improvement of fracture toughness and other mechanical properties such as modulus, strength, stiffness. Factors influencing the potential of nanoreinforcement for the enhancement of the damage resistance of polymers include, on one hand, the structural parameters of nano-particles, like aspect ratio [12–15], hardness [13,16–18] and shape [16], and on the other hand, the morphology of nano-particles in matrix, such

* Corresponding authors.
E-mail addresses: ggda@dtu.dk (G. Dai), lemi@dtu.dk (L. Mishnaevsky Jr.).

0266-3538/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compscitech.2012.10.003

as orientation [12], clustering [17,19] and weight content [12–21]. In fact, the reduction of nanoplatelets aspect ratio leads to the lower modulus and yield stress, but also to an improvement in fracture toughness [12,19]; soft nano-particles (such as rubber) have a positive effect on the fracture toughness of nanocomposites (as differed from hard particles). With view on the effect of nanoparticle elastic properties, it was observed that an addition of hard nano-particles improves the elastic modulus of nanocomposite (as can be expected), while soft nano-particles have a negative effect on the elastic properties [17,18]. Spherical nano-particles demonstrate a weaker toughening effect than the plate-like nano-particles [16].

The morphology of the nano-particle distribution in the matrix is another factor that influences the damage mechanisms and mechanical properties of nanocomposites. It was found that aligned nanoparticle arrangement leads to a significant improvement in the elastic modulus but also to the reduction of fracture toughness [12]. The clustering of nano-particles in matrix, mainly described in term of exfoliation or intercalation, affects the fracture toughness and modulus differently. A well-dispersed distribution of nano-particles in matrix results in a significant improvement in the elastic properties but leads to the decrease of toughness [20]. The weight content of nano-particles, which is considered the most important factor, is taken into account in a number of research works [12–14,16–21]. Conclusions are made that the modulus and the tensile strength will monotonously increase and decrease, respectively, as the nano-particle weight content increases; the toughness of nanocomposites shows a maximum value at the weight content of 2.5% [20].

3. Computational model: 3D multiplatelets model

In order to simulate the damage mechanisms of nanoclay-reinforced polymers, a series of four phases 3D multiplatelets model with effective interface surrounding or located between the nanoplatelets has been developed for various types of microstructures. Different models of nanocomposites (varying in nanoplatelets aspect ratio, dispersion, orientation and weight content, etc.), which can be generated automatically with the use of the Python based code "3DNanoDisk", are developed in this work. Computational experiments have been carried out to analyze the effect of the nanoplatelets and their distribution on the deformation and damage mechanisms in the nanocomposites.

3.1. Nanoreinforcement: effective interface concept

Since the traditional micromechanical models do not reflect the real influence of nanoreinforcement on the mechanical properties and strength of polymers, the "effective interface" concept has been suggested and used in many works [7,22–24]. Odegard et al. [7] introduced the finite size "effective interface" layer to replace the interfacial regions between the polyimide and nanoparticle because of the drawback of Mori–Tanaka approach on simulating the mechanical performance of nano-structured reinforcement. The nanometer level reinforcement and adjacent polymer region is well described by the "three phase model". Recently, Wang et al. [24] generalized the "effective interface" as one outside stiffer layer in conjunction with another inside softer layer and proved it was valid as the particles interfered in each other because of the high weight content of nanoplatelets.

In order to take into account different compositions and properties of the interfacial regions located between closely arranged platelets and the regions surrounding the platelets or clusters [24] and following the analytical model [9], the former "three phase" model is generalized by including the "fourth phase" which is named the "'intrastack interphase'". In this case, the model consists of matrix, nanoplatelets, the "coating phase", surrounding single platelets in exfoliated structures or clusters in intercalated structures, respectively and the "'intrastack interphase'", lying between clustering nanoplatelets. As noted in [9], the intrastack phase has lower critical damage level than the usual interface.

3.2. Automatic generation of 3D unit cell with high aspect ratio disk-shaped nanoplatelets

A special Python based code was developed, which allows generating 3D multielement FE models of nanocomposites with high aspect ratio particles, varied orientations and volume contents, and, in particular, with nanoparticles surrounded by coatings and/or intrastack phases. This program allows also to vary the particle distribution, e.g. clustering (intercalation and exfoliation of nanoplatelets) and the orientation (ordered or disordered) of

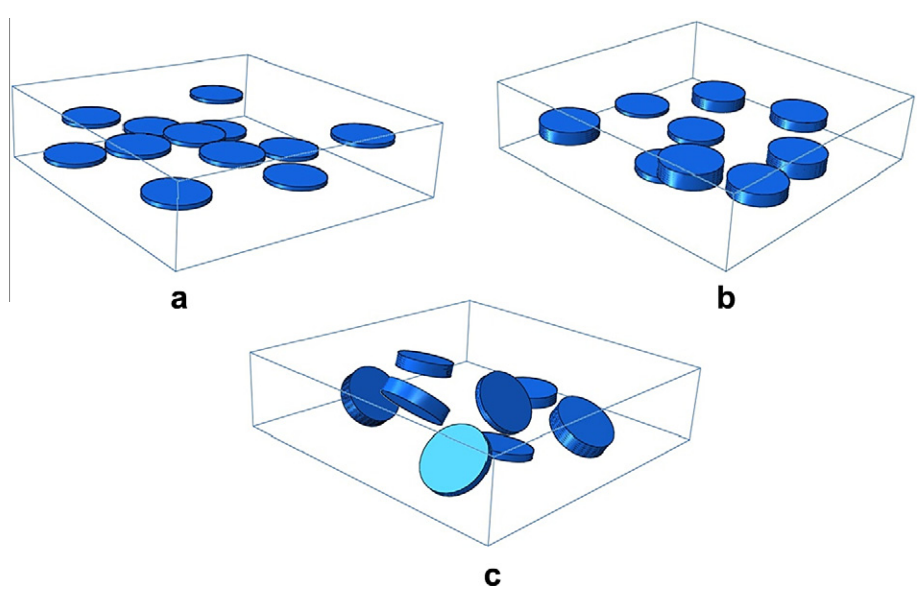

Fig. 1. Examples of 3D models of nanocomposites with different arrangements of nanoplatelets. (a) Unit cell with aligned horizontal exfoliated nanoplatelets. (b) Unit cell with aligned multi-clusters. (c) Unit cell with randomly oriented clusters.