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Finite element prediction of stress transfer in graphene nanocomposites: The interface effect

K.N. Spanos, N.K. Anifantis *

Mechanical and Aeronautics Engineering Department, University of Patras, 26500 Rio, Patras, Greece

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ABSTRACT

A micromechanical hybrid finite element approach is implemented in this study, in order to evaluate the stress transfer characteristics in graphene-based nanocomposites. Three-dimensional representative volume elements, consisting of two different parts, have been used during the analysis. The matrix material that is modeled as continuum (solid finite elements), and the graphene sheet that is modeled discretely (spring based elements). Between these two constituents, an interfacial region is taking place, simulated by appropriate stiffness variations, defining a heterogeneous region that affects the stress transfer behavior of the composite. Our simulations show good agreement with existing studies of the open literature and indicate the effect of a number of factors in stress transfer efficiency.

1. Introduction

Nowadays, nanocomposites are widely used due to the broad range of possibilities and options they present. They provide increased mechanical, thermal, electrical and magnetic properties, without sacrificing the processability of the matrix material, the initial mechanical properties and its light weight. They can be utilized in aerospace and in automotive as structural materials, and in electronics as sensors or other components. Carbon nanotubes (CNT), which are the best known and most widely used component of nanocomposites have been investigated, as reinforcements, to the utmost [1–3]. However, their high cost and the weakness to concentrate, sufficient amounts of nanotubes, in an easy way, turned the researchers in the seek of alternative reinforcing materials [4,5]. Some nanomaterials that could be used as reinforcements in nanocomposites are the platelets, such as exfoliated nanoclays [6,7], graphene platelets [8] and chemically treated graphene oxide [9]. Another alternate component in nanocomposites is graphene. Graphene is much cheaper than carbon nanotubes, can be found in large amounts from a graphite precursor and has superb properties. It has been found that graphene has a Young's modulus on the order of 1 TPa and an intrinsic strength of around 130 GPa. [10]. Pristine graphene can also be made by mechanical exfoliation of graphite in organic solvents [11]. Having all these advantages, as reinforcing material, it has become a promising solution in nanocomposites production, with similar or even better performance than the CNTs [12–14].

Difficulty in the dispersibility of the reinforcing material and proper interfacial stress transfer are the major problems encountered in the nanocomposites study. The mechanical properties of the combined materials, the surface of the fiber (graphene), and the nature of the fiber/resin bonding as well as the effective interfacial stress transfer are the primary factors that will affect the mechanical characteristics of a composite. Among them, the adhesion between the fiber and the matrix is a dominant parameter. The improvement of the mechanical properties of a composite material is affected by the mechanical properties of the interface, i.e. the ability to transfer stresses sufficiently. [15–20]. Interface of a composite, in micromechanics, is a zone of varying width, consisting of the structural and compositional components of the composite, and sharing similar properties with it. It represents the chemical bonds and van der Waals interactions between the graphene and the matrix. An efficient coupling between reinforcement and matrix is essential for the stress transfer at the interface. Thus, the way of measuring the qualitative characteristics of interfacial stress transfer between graphene and matrix is an important issue. However, most studies have focused more on finding essential properties of nanocomposites and less on finding the local load-transfer characteristics at the interface.

In order to understand the load transfer conditions various researchers have made some experimental studies mainly using the Raman Spectroscopy method. This method can be used to follow the stress transfer in a variety of composites reinforced with

* Corresponding author.
E-mail address: nanif@mech.upatras.gr (N.K. Anifantis).

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carbon–based materials [21,22]. Cao et al. [23] found that the covalent bonding promotes the efficient stress transfer from the matrix to the reinforcement, and thus enhances the mechanical properties of the resulting composites. Cai et al. [24] found that the chemical bonds were formed between the graphene sheets and PU matrix, which made a big contribution to stress transfer. Using the same method, Gong et al. [25] demonstrated that graphene bilayer is not the best material to be used as a basis for strengthening nanocomposites. Good stress transfer from the matrix to the bilayer graphene may exist only when it is completely encapsulated in the polymer matrix. Then, there is no slippage between the two layers. Less effective stress transfer has been observed when examining trilayer or multilayer graphene due to sliding between the inner layers of graphene. On the other hand, in these last cases, higher volume fractions may be achieved.

An analytical method made by Zhang et al. [26] presented similar results. Studying the case of graphene nanosheet (GNS) reinforced hydroxyapatite (HA) composite, they found that the number of graphene layers of the added GNSs has little effect on the maximum axial stress (0.35 GPa) and the maximum shear stress (0.14 GPa) at a GNS-HA interface, and the energy dissipation by GNS pull-out decreases with increasing the number of graphene layers due to weak bonding between them.

Another experimental study was made by Feng et al. [27]. They studied the reduced graphene oxide (rGO)/PVA composites. They found that the specific interactions between the components, such as the force of the hydrogen bonding, significantly improved the rGO-based composites. Furthermore, graphene sheets have high surface to volume ratios owing to the accessibility of the atomically thin 2D surface to polymer molecules, which makes graphene sheets potentially more favorable for altering all matrix mechanical properties.

Using molecular dynamics simulation Zhang et al. [28] investigated the interfacial load transfer and the region between graphene and matrix. They claimed that another phase of polymer matrix is developed around the graphene and CNT with certain thickness and is termed as "interphase zone". These regions were found to have higher density and strength compared to the normal polymer matrix. The detachment always locates at the polymer matrix, as the damage path always avoids the stiff "interphase zone". Awasthi et al. [29] used the same method investigating the separation in sliding mode together with normal loading and size dependence in order to obtain limiting behavior in the force displacement responses. They also found that mechanical interactions between graphene and polymer chains are stronger than those among the polymer chains. During the separation process, a few polymer chains, particularly those near the graphene surface, stayed adhered to graphene and slipped away from the remaining polymer.

In this present study, we use a computational model to properly evaluate the load transfer characteristics of graphene-reinforced nanocomposites. A basic rectangular representative volume element has been proposed for the modeling. The three dimensional atomistic microstructure of the graphene is utilized [30], when the matrix material is assumed as continuum. The interface is simulated by special joint elements of variable stiffness that interconnect the matrix with its reinforcement. In this way, a heterogeneous interface is created that enables and permits a smoother transition between the two materials of such irrelevant stiffnesses. The computational cost and the modeling complexity were significantly reduced due to the hybrid approach, enabled by this macroscopic representation of the constituents. Thus, possible covalent bonding and van der Waals interactions between the two phases is avoided. The proposed formulation has been extensively presented by authors in a previously published work [31]. This formulation is also implemented here and is mentioned, in less detail, for reasons of completeness. Parametric investigation, concerning the interfacial stiffness, the graphene geometry and volume fraction, and the matrix material stiffness has been conducted and its results are presented and evaluated.

2. Materials and methods

In the present study appropriate representative volume elements (RVEs) are implemented for the description of the computational model. The computational model consists of three parts, each of which is modeled differently. The graphene sheet is modeled in nanoscale, implementing a structural model, based on the molecular mechanics theory. The matrix material is modeled in macroscale, using convenient finite element modeling. The interface between them is of great importance and is the leading object of this study since it affects the stress transfer. Here, the interfacial region, based on the macroscale mechanical properties of the graphene sheet and the matrix material, is model discretely.

2.1. Micromechanical analysis

Primarily, the representative volume element is a short-length graphene sheet embedded in the matrix material. Thus, the graphene length L_g and width W_g will be smaller than the total length L_c and width W_c of the RVE, respectively. A long-length graphene sheet is used as reinforcement, i.e. the graphene sheet has the same length with the matrix and will be examined for comparison reasons. Its orientation is not random but it is aligned and continuous in the polymer. It has a sandwich-like geometry, consisting of two phases, i.e. the graphene sheet and the matrix. These phases are linked together via an interfacial region. The length of the RVE, in this case, is equal to the graphene length and to the matrix length L_m. The matrix width W_m is equal to the graphene width, equal to the total width of the composite. The graphene thickness t_g coincides with the interfacial theoretical thickness t_i, and together with the matrix thickness t_m, both divided in two equal parts, $t_g/2$ and $t_m/2$, respectively, they compose the total thickness t_c of the RVE. According to the RVEs employed here (Figs. 1 and 2), the volume fraction of the graphene sheet within the composite is expressed by:

$$V_{fr} = \frac{V_g}{V_m + V_g}. \tag{1}$$

where V_m and V_g are the volumes of the matrix and graphene respectively. Small volume fractions are considered, so that a negligible interaction between adjacent graphene sheets can be assumed. These equations show that, with constant graphene geometry, different volume fractions can only be achieved by

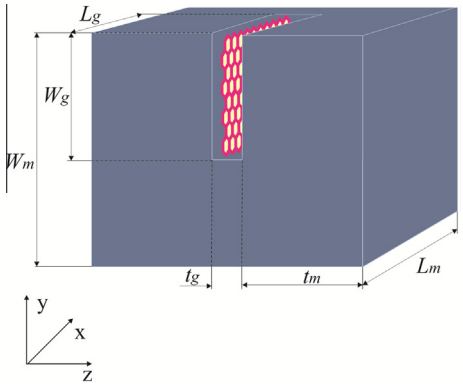

Fig. 1. The RVE of graphene based composite (Embedded type).