Modelling of interface stress transfer in graphene monolayer nanocomposites under static extension load

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Abstract. An investigation on the interfacial stress transfer in nanocomposite between a monolayer of graphene and a common size polyethylene terephthalate (PET) matrix under extensional traction applied to the matrix is presented. The constitutive law describing the behaviour of the interface is assumed to be a bi-linear cohesive one. Three zones are defined along the interface: elastic, cohesive and delaminated. The system of ordinary differential shear lag equations together with boundary, symmetric and continuity conditions is solved consequently at each zone and the respective solutions are fitted at common points. The values of these common points – the ends of the lengths of the elastic, cohesive and delaminated zones are determined using the solutions of two nonlinear algebraic system equations about them. All results are illustrated in figures and discussed in detail. A comparison of the results obtained with the model considered and experimental data is done and confirms that for the structure of a length 21.8 nm the interface delamination is not observed. The implemented method offers a simple tool to understand the nature of the interface behaviour and evaluation of the damaging of the nanostructure.

1 Introduction

Graphene is a monolayer of honeycomb lattice of carbon atoms discovered in 2004. The research communities have shown a lot of interest in this novel material and its unique properties. As a consequence, the publications on graphene have dramatically increased in recent years. Graphene is also one of the stiffest (modulus ~1 TPa) and the strongest (strength ~100 GPa) material with thermal conductivity (~5000 W/mK). Based on these exceptional properties, graphene has found its applications in various fields such as sensors, electrodes, solar cells, energy storage devices and nanocomposites. Therefore, graphene-polymer nanocomposites have demonstrated a great potential to serve as next generation functional or structural materials.

Over the last decades, a variety of numerical and analytical models has been developed to investigate the behavior of monolayer graphene nanocomposites. Recently, the shear lag method which is 1-D analytical method has been widely used in many engineering problems related with interface stress transfer and delamination [1-14].
From mathematical point of view, the shear-lag model is the simplest of 1-D analytical model, used for the stress transfer analysis in unidirectional composites. This model is based on a simple differential equation which relates the fiber axial stress to the interfacial shear stress. It is not applicable at higher volume fractions due to the significant interactions of fibers. Also, the model cannot predict changes of axial stress and strain distributions in the radial direction. As a result, due to these limitations, the shear-lag model cannot provide reliable predictions for the composite properties, and thus, its application for short fiber composites has been limited overtime.

In the present work the bi-linear shear stress is implemented in shear lag analysis for a monolayer graphene/PET nanocomposite. The representative model unit consists of two layers (graphene hosted on substrate of PET is considered). The substrate is loaded by axial traction on extension. As a consequence the statements as well as the boundary and continuity conditions are given in tractions. Three zones are defined along the interface: elastic, cohesive and delaminated. The respective solutions are fitted using continuity conditions. The system of two nonlinear algebraic equations gives a possibility to find the lengths of the elastic and cohesive zone. The obtained results are illustrated in figures and discussed. A comparison with experimental results [13] shows that the used method is sufficiently good to give a quick prognosis for the damaged composite.

2 Statement of the problem
The representative model unit of the structure and the interface shear stress behaviour are presented in Figure 1(a) and (b), respectively, where the layer A is traction free and the layer B is loaded by an extensional traction $T$. The parameters $h_A << h_B, E_A, E_B$ are the layers thicknesses and elastic moduli, respectively. The modified shear lag analysis will be applied to the considered structure. The interface $l$ works only on shear, bending is neglected. The coordinate system $Ox_z$ is placed in the middle of the structure with a length $2l$. Due to the symmetry, only half of the structure will be considered.

![Figure 1](image-url)

Figure 1. Representative unit of graphene monolayer nanocomposite (a) and interface shear stress behaviour (b)

The following shear lag equations for the model hold:

$$\frac{dT_A}{dx} = 2h_A \frac{d\sigma_A}{dx} = \tau_I \quad ; \quad \frac{dT_B}{dx} = 2h_B \frac{d\sigma_B}{dx} = -\tau_I$$

$$T_A(x) = 2h_A \sigma_A \quad ; \quad T_B(x) = 2h_B \sigma_B \quad ; \quad \varepsilon_A(x) = u'_A \quad ; \quad \varepsilon_B(x) = u'_B \quad ; \quad u_I = u_A - u_B$$

For interface shear stress $\tau_I$ we assume:

$$G_I \frac{u_I}{h_I} = K_I u_I \quad for \quad u_I \leq u'_I = \frac{\tau_I}{K_I}$$

$$\tau_I = \frac{\tau'_I}{h_I} = \frac{K_I}{h_I} \left( u_I - u'_I \right) = \frac{\tau'_I - K_I u_I}{h_I} \quad for \quad u_I > u'_I \quad ; \quad u'_I = \frac{\tau_I}{K_I} \left( \frac{1}{K_I} + \frac{1}{K_I} \right)$$

$$0 \quad for \quad u_I \geq u'_I$$

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Here interface thickness is $h_I$, and $K_{II}, K_s$ are effective elastic shear and softening moduli of the interface bonding layer. The plate $B$ is under extension $T = 2h_B E_B e_0$, plate $A$ is free. The interface $I$ is also assumed linear elastic, working only on shear. During the monotonically increasing traction $T$ and due to the assumed interface stress behaviour in equation (2), three zones can be defined along the length of the interface $l$ (see Figure 1(b)). Along the first zone the elastic behaviour for the interface is valid. The interface remains continuous until reaching the critical value of interface shear stress $\tau_I = \tau^c_I$ at both ends of the structure. The length of the pure elastic zone is $l_e$.

Let the length of the softening zone be $l_d$. The softening zone follows the cohesive law for the interface shear stress, where $\tau_I > \tau^c_I$. This zone will be called “cohesive” (damaged) zone. The proper continuity conditions should be stated to match different stress and displacement regimes at transition point $l_e$ with length $(l_d - l_e)$ between the elastic and softening zones.

The third zone consists of pure delamination of the interface and then $\tau_I = 0$. At the same time, the proper continuity conditions at transition point $l_d$ (length of this zone) should be stated.

In all three zones the stress interface behaviour is determined, satisfying the BC and proper continuity conditions. Finally, the lengths of both transition points $l_e$ and $l_d$ are calculated. The boundary, symmetry and continuity conditions for the solutions in three zones are:

### Elastic zone - $0 \leq x \leq l_e$

- $T_E^A(l_e) = 0$
- $\tau_E^I(l_e) = -\tau_I^c$
- $\tau_E^I(0) = 0$
- $T_E^d(l_e) = T$

### Softening zone - $l_e \leq x \leq l_d$

- $T_E^A(l_e) = 0$
- $\tau_E^I(l_e) = 0$
- $\tau_E^I(0) = 0$
- $T_E^d(l_e) = 0$

### Delamination zone - $l_d \leq x \leq l$

- $T_E^A = 0$
- $\tau_E^I = 0$
- $T_E^d = T$

For simplicity, the analytical solutions in all three zones are calculated and briefly given below only for interface shear stresses, tractions and deformations, taking into account the following notations:

\[
\lambda^2 = \left(\frac{1}{2h_A E_A} + \frac{1}{2h_B E_B}\right) K_I; \quad \rho = \frac{2h_A E_A}{2h_B E_B}; \quad \lambda^2 = \left(\frac{1}{2h_A E_A} + \frac{1}{2h_B E_B}\right) K_s \\
F = \left(\frac{1}{2h_A E_A} + \frac{1}{2h_B E_B}\right) \left[1 + \frac{K_s}{K_I}\right] \tau_I^c = \frac{\lambda^2}{K_s} \left[1 + \frac{K_s}{K_I}\right] \tau_I^c
\]

#### Elastic zone: $0 \leq x \leq l_e$

- $\frac{d^2 u_I}{dx^2} = \lambda^2 u_I$

Solutions:

\[
\tau_I^c(x) = -\frac{\sinh(\lambda x)}{\sinh(\lambda l - x)}; \quad T_E^A(x) = -\frac{\tau_I^c(x)}{\lambda} \cosh(\lambda x); \quad T_E^d(x) = T_E^A(x)/(2h_A E_A)
\]

#### Softening zone: $l_e \leq x \leq l_d$

- $\lambda^2 = \lambda^2 u_I + F$

Solutions:

\[
\tau_I^c(x) = -\frac{\rho}{1+\rho} T \lambda \sin(\lambda (l_d - x)); \quad T_E^A(x) = \frac{\rho}{1+\rho} T [1 - \cos(\lambda (l_d - x))]; \quad T_E^d(x) = T_E^A(x)/(2h_A E_A)
\]

#### Delamination zone: $l_d \leq x \leq l$

- $T_E^A(x) = 0; \quad T_E^d(x) = 0; \quad \epsilon_E^A(x) = 0$

For determination of zones lengths $(l_e, l_d)$ it is required that: $\tau_I^c(l_e) = -\tau_I^c$ and $T_E^A(l_e) - T_E^A(l_e) = 0$, or:
\[ l_d = l_e + \frac{1}{\lambda_s} \arctg \left[ \frac{\lambda_s}{\lambda_a} \coth(\lambda_a l_e) \right]; \quad T = \frac{\tau^*}{\lambda_a} + 1 + \frac{\rho}{\lambda_a} \coth(\lambda_a l_e) \left[ 1 + \frac{\lambda_s}{\lambda_a} \tanh(\lambda_a l_e) \right]^{1/2} \] (6)

3 Numerical example and discussion

Material properties and geometry of the considered nanostructure in Figure 1 are taken from [13] and are presented in Table 1. For pure elastic zone over the whole graphene length of 21.8 μm it can be obtained an additional equation (7) for model strain, derived from last equation in Equation (3) at \( l_e = l \) (the same result is obtained in [11]):

\[ \varepsilon^*_A(x) = \frac{T \rho}{2h_A E_A (1 + \rho)} \left[ \frac{\cosh(\lambda_a x)}{\cosh(\lambda_a l)} \right] \] (7)

This equation is used to make a comparison is between our results for this strain and experimental data in [13,14] for graphene length of 21.8 μm. The comparison is presented in Figure 2 and the model results fit well with experimental data, both for two different external uniaxial loads (\( \varepsilon_0 = 0.4\% \) and 0.6%, which correspond to applied tractions \( T = 42 \) and 63 kN/m, respectively).

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|  |   |   |   |   |   |   |

Table 1. Material properties and geometry of considered structure

\begin{tabular}{cccccccc}
\hline
\textbf{\( E_A \)} & \textbf{\( E_B \)} & \textbf{\( K_I \)} & \textbf{\( K_{II} \)} & \textbf{\( \tau_f^* \)} & \textbf{\( 2h_A \)} & \textbf{\( 2h_B \)} & \textbf{\( 2l \)}
\hline
TPa & GPa & TPa/m & TPa/m & MPa & nm & m & μm
\hline
1 & 3 & 74 & 1.596 & 0.5 & 0.35 & 0.35e-04 & 21.8;60
\hline
\end{tabular}

Figure 2. Comparison between experimental data in [13] and results obtained from equation (7) for the strain in graphene along the graphene length 21.8 μm only, at two different external uniaxial loads (\( \varepsilon_0 = 0.4\% \) and 0.6%).

In Figure 3(a), the axial strain \( \varepsilon_A(x) \) is shown for five values of the external tractions in all three zones – elastic, softening and delamination (equations (3)÷(5)), and in Figure 3(b) the behaviour of the interfacial shear stress in all three zones at the same external loadings is shown. For simplicity, in Figure 3(a) and 3(b) only the essential part of the length \( 2l = 60 \) μm is presented.

It can be seen that increasing the load, maximal values of \( \varepsilon_A(x) \) decrease and delamination increases. This also confirms the non-linear cohesive shear lag model observations in [13] in the sliding region for strain in graphene. The character of the curves for \( \tau_f(x) \) changes as the applied load increases (at
Figure 3(b) – up to 1% there is still a small plateau in the middle of graphene length, like in [13], after 2% the bi-linear cohesive behaviour is well visible. The cohesive behaviour described in equations (3-5) occurs at graphene length 60 \( \mu \text{m} \) after 0.025%, at which the obtained lengths of elastic and cohesive zones are 5.1883e-07m and 1.546e-05m, respectively. At loads less than 0.025% no real roots \((l_e, l_d)\) of equation (6) are obtained.

In Table 2 the results obtained from equation (6) for the lengths \((l_e, l_d)\) are given at different loading tractions for graphene length of 60 \( \mu \text{m} \).

![Graph](image)

**Figure 3.** The axial strain \( \epsilon_A(x) \) in graphene along the graphene length, for various external uniaxial tractions (a), and interfacial shear stress \( \tau_I(x) \) along the graphene length, for various external uniaxial tractions (b)

| \( \tau \) (kN/m) | 31.5 | 52.5 | 105 | 210 | 315 |
|-----------------|------|------|-----|-----|-----|
| \( \epsilon_0 \) (%) | 0.3  | 0.5  | 1   | 2   | 3   |
| \( l_e \) (m)     | 2.2579e-8 | 1.3525e-8 | 6.7582e-9 | 3.3785e-9 | 2.2523e-9 |
| \( l_d \) (m)     | 1.0674e-6 | 6.4012e-07 | 3.1998e-7 | 1.5998e-7 | 1.0665e-7 |

4 Conclusions

In this work the modelling of interfacial stress transfer in a nanocomposite between graphene monolayer and a common size polyethylene terephthalate (PET) matrix under extensional traction applied to the matrix is presented. The constitutive law describing the behaviour of the interface is assumed to be a bi-linear cohesive one. Three zones are defined along the interface: elastic, cohesive and delaminated. The system of ODE shear lag together with boundary, symmetry and continuity conditions is solved consequently at each zone and the respective solutions are fitted at common points. The values of these common points - the ends of the lengths of the elastic, cohesive and delaminated zones are determined using the solutions of two nonlinear algebraic system equations about them. A comparison of the model strain results in graphene and experimental data of [13] is done and confirms that for the structure of a length 21.8 \( \mu \text{m} \) the interface delamination is not observed. For graphene length of 60 \( \mu \text{m} \) after parametric analysis it was found, that increasing the external load, the maximal values of strain at the centre of graphene for all three zones solutions decrease and delamination increases. At graphene length of 60 \( \mu \text{m} \) the interfacial shear stress also follows the predicted cohesive bi-linear behaviour, and delamination increases with applied load increasing.
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