



Deformation mechanism of graphene in amorphous polyethylene: A molecular dynamics based study



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ABSTRACT

The current paper focuses on investigating deformation mechanism of graphene sheets in a graphene reinforced polyethylene (Gn-PE) nanocomposite. Classical molecular dynamics (MD) simulation was conducted on large Gn-PE systems. Different spatial arrangements of graphene sheets were considered in order to study the effect of nonlocal interaction among the graphenes. In all the cases 5% weight concentration of graphene was considered in order to prepare atomistic models for Gn-PE. As expected, graphene seemed to enhance the overall Young's modulus and tensile strength of the Gn-PE nanocomposite. Randomly oriented graphenes with strong nonlocal interaction were observed to be comparatively preferable than the other spatial arrangements of graphenes. The high strength and stiffness of graphene sheets can be properly utilized if the graphenes are randomly oriented and have strong long range interactions. Finally, the failure mechanism of the graphene and role of voids in the polymer were discussed both qualitatively and quantitatively. It was seen that the randomly oriented graphenes were firstly pulled out from the polyethylene matrix during deformation prior to breaking into pieces. This can explain the loss of stiffness and strength in graphene sheets embedded in the polymer matrix. From the current work it is clearly understood that the necessity of the long range graphene-graphene interaction is important in both elastic as well as plastic regime of the deformation.

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1. Introduction

Polyethylene (PE) is one of the most widely used polymers in variety of structural applications due to its light weight, low cost and good mechanical properties. After processing, PE molecules remain in amorphous as well as crystalline phases. The amorphous phase is present in both low density polyethylene (LDPE) or semi-crystalline high density polyethylene (HDPE). Higher volume fraction of crystalline phase leads to higher mechanical stiffness and the amorphous phase increases the flexibility. The amorphous phase is complex and challenging to analyze. So the current work focuses on investigating the amorphous phase of PE. Due to highly increasing applications of PE it has been necessary to enhance the mechanical, thermal and electrical properties of the PE. In this regard researchers have been incorporating nano-fillers in PE. Recent studies showed that properties of PE were enhanced by embedding clay, carbon-nanotubes (CNTs), carbon-nanofibers or graphites in the polymer by preparing polyethylene-nanocomposites [1]. Graphite is a nano-material composed of stacked 2D graphene

nano-platelets (GNPs). The Young's modulus of the GNP is approximately 1.0 TPa. The mechanical properties of graphene is very close to the carbon nanotubes. GNPs are obtained from graphite by exfoliation using ultrasonication method [2]. Compared to CNTs, graphite is cost effective. So GNP reinforced PE nanocomposite has drawn attention to the scientific community as a potential key material for different structural applications.

In past few years researchers have been investigating the effect of incorporating GNP in PE. Several experimental works have been done in order to evaluate the change in mechanical, thermal and electrical properties of PE reinforced by graphenes [1–4]. It was seen that graphene reinforced PE nanocomposites (Gn-PE) have better mechanical properties compared to neat PE. Graphene seems to be a promising nano-filler material for both LDPE and HDPE. However, it is experimentally quite challenging to investigate the mechanism of graphene deformation in Gn-PE nanocomposites at the atomistic level. In order to improve the properties of Gn-PE it is very important to study the deformation mechanism of graphene in presence of the host polymer PE. Primarily, graphenes stay in the PE matrix in two phases [1]. In one case the nonlocal interaction between the graphenes is not well enough to increase the stiffness. Graphenes need to be well dispersed in the PE matrix

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in order to have better load transfer from PE. A thorough investigation is necessary to make a clear understanding on the effect of spatial arrangement of graphenes. This demands for a detail theoretical investigation using state-of-art computational modeling schemes. Classical molecular dynamics (MD) simulation has been a reliable tool for performing investigation on material deformation at atomistic scale. There are significant research works have been carried out on amorphous PE using MD simulation [5–7]. In these papers, besides calculating elastic properties, MD simulation was used to analyze the deformation mechanism of PE molecules under uniaxial tensile deformation. Although deformation and failure of pristine graphene sheets were analyzed using MD simulation [8], research related to atomistic scale investigation of graphene deformation in Gn–PE has not been noticed in the literature. In the presence of host polymer (PE), graphene may deform in a different manner considering the inter-molecular interactions between graphene and the PE molecules. Hence, it is not a trivial task to establish a clear understanding on the deformation mechanism of graphenes embedded in PE.

In the current paper, MD simulations were carried out on Gn–PE models with 5% graphenes in order to investigate the deformation, failure and interfacial debonding of graphene sheet in Gn–PE nanocomposites. The effect of spatial arrangement of graphene sheets on the elastic properties and deformation of graphene has been thoroughly discussed.

2. Computational scheme

Prior to conducting molecular dynamics simulation, the initial structures of Gn–PE models were needed to be prepared. Graphene sheets with length = 211.62 Å and width = 9.84 Å were considered as nano-fillers for the amorphous polyethylene. Five graphene sheets were embedded in each cubic unitcell in order to maintain 5% weight concentration in the polymer. Mainly, two types of Gn–PE systems were considered based on graphene's spatial arrangement. One is with randomly oriented graphene sheets and another

one is stacked graphene sheets. The randomly oriented graphene sheets in polymer matrix leads to dispersed graphene based polymer nanocomposites. However, the dispersion quality should be optimum in order to ensure better nonlocal interaction among graphene sheets as well as graphene and polymer matrix. As shown in Fig. 1(a–c) the long range interaction among the randomly oriented graphenes can be reduced by dispersing them far enough so that they interact with the polymer almost independently. This may cause poor load transfer between polymer matrix and graphene sheets. On the other hand, the stacked graphenes (Fig. 1(d)) affect the load transfer mechanism in a different way. So, these Gn–PE systems were considered to investigate the effect of graphene arrangement on the overall mechanical properties and load transfer quality.

Each Gn–PE system contains 248,142 atoms among which 4990 atoms belong to five graphene sheets. The spatial arrangements of the graphenes are shown in Fig. 1. The Gn–PE containing randomly oriented graphenes with strong and weak nonlocal interactions are named as Gn–PE:A, Gn–PE:B and Gn–PE:C, respectively. Gn–PE:A and Gn–PE:B are based on Fig. 1a and b, respectively. In both of the cases the nonlocal interaction among graphene is better than in Gn–PE:C. On the other hand, the stacked graphene based system is named as Gn–PE:D. The average volume of the cubic unitcells varied between $18.6 \times 10^6 \sim 19.93 \times 10^6 \text{ Å}^3$. Different Gn–PE systems are shown in Fig. 2. Graphene sheets were embedded into the polymer matrix which was generated by randomly distributing PE molecules in a cubic unitcell. Each PE molecule contains 182 atoms. The maximum distance between two graphene sheets was 93.5 Å and 148.683 Å in Gn–PE:A and Gn–PE:C, respectively. This is 16.72 Å in Gn–PE:D. For Gn–PE:A the maximum distance was calculated from tip of one graphene to the tip of another graphene. Given the critical length scale for amorphous PE is approximately 300 Å [9], the large inter-graphene maximum distance in Gn–PE:B leads to less nonlocal interaction as beyond 300 Å the nonlocality in amorphous PE is reduced.

This current work is divided into two major components. Firstly, after embedding the graphenes, each system was equilibrated using MD steps preceded by energy minimization. Polymer

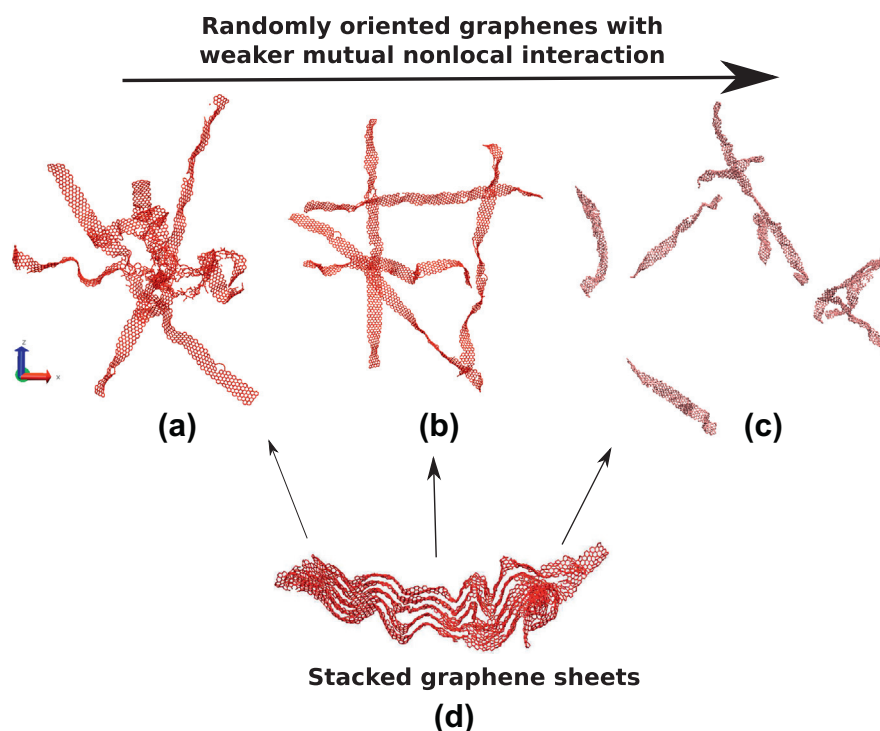


Fig. 1. Different spatial arrangements of graphene sheets.

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