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Elastic and fracture characteristics of graphene-silicon nanosheet composites using nonlinear finite element method

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ABSTRACT

A simple and efficient methodology is proposed for computing the nonlinear stress-strain behavior and fracture strength under tensile loading of graphene-silicon nanosheet composites. A nonlinear finite-element model (FEM) is developed to obtain the stress-strain relationships, which in general are computed using the computationally expensive procedure of molecular dynamics (MD) simulations. The modelling method, based on the interconnection of continuum micro-mechanics approaches, incorporates bonded contact at the graphene-silicon interface with the graphene being modelled as the multilinear elastic and the silicon assumed as an isotropic material is fed into an atomistic progressive fracture model. Using this model, we get the nonlinear behaviour of graphene, silicon and its composites, as a nonlinear stress-strain curve with their critical stress at inflection point leading to failure. The obtained results of the stress-strain curves, the elastic modulus and the critical stresses of single layer graphene (SLG), silicon nanosheet and their composites (GSNC) with different thickness of silicon nanosheet are in good agreement with the MD results available in the literature. These results elucidate that the tensile strength and Young's modulus of the silicon nanosheet increase enormously by putting the graphene layer on the top and bottom surface of the silicon nanosheet. This model is then employed to study the non-linear stress behaviour for the different orientations of silicon with varying thickness and their corresponding composites with graphene and the effect of various chirality of SLGs are also considered. Thus, we try to establish FEM as a reliable numerical method to obtain the mechanical behaviour of graphene-silicon nanosheet composites which for long-time has been solved using the classical approach of MD. The parametric study which is done using the developed FEM model shows that the GSNC helps to enhance the mechanical properties of silicon nanosheet, which in turn is helpful for the silicon-based semiconductor industry. This fact correlates well with the other methods, well-established in the literature.

1. Introduction

Graphene and its composites have various application in the field of aerospace, bio-electric sensors [1], bio-engineering [2], electronics [3], energy technology, lithium batteries [4], and different other fields of nanotechnology due to their excellent electrical, mechanical and thermal properties [3,5]. Single layer graphene (SLG) needs an appropriate supporting substrate which should either not disturb the amazing properties of graphene or enhance the properties of the hybrid graphene and its substrate system. Moreover, enlargement of graphene-based composite devices and growth of their structures demand an in-depth understanding of combined properties of graphene and its supporting element. The silicon nanofilm has been the most commonly preferred material in the area of nano- and micro-electromechanical systems (NEMS/MEMS) because of its integration compatibility with microelectronic circuits [6], which make it advisable to incorporate into miniaturised systems for portable applications. To further widen the application of silicon nanofilm to change the band gap or make a more sensitive diode, transistor or other such devices, researchers have proposed placing a graphene layer on top of the silicon film to form graphene-silicon nanosheet composites (GSNC). In this paper, we have systematically analyzed the elastic and fracture properties of GSNC with SLG on single or both sides of a silicon film to make the device reliable.

To analyze graphene composites, molecular dynamic simulation and finite element based multiscale approaches have been successfully developed and presented in the literature [7–14]. Cho et al. [7] have done a multi-scale analysis to find the mechanical properties of graphite/epoxy nanocomposites using the Mori–Tanaka approach in conjunction with molecular mechanics. Tserpes et al. [8] have developed a multiscale model for unidirectional nanotube/polymer composite based on continuum elasticity. They have proposed separate models for CNT and polymer matrix. They have demonstrated that a proper adhesion provides the maximum load carrying capacity from polymer to the CNT. Montaz-

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eri et al. [9] have provided a full investigation of the mechanical properties of graphene-based nanocomposites using molecular structural mechanics/finite element (MSM/FE) multiscale modelling approach to study the effect of GS inclusions on Young's modulus of the polymer matrix. They have also compared the elastic constants of CNT-reinforced and GS-reinforced polymer composite. GS-polymer interaction is modelled using nonlinear spring elements to couple GS and polymer phase. Chandra et al. [12] have also described a multiscale approach to simulate the tensile properties of graphene-reinforced nanocomposites using a FE atomistic model represented by higher order Timoshenko beam elements for the graphene system. They have represented the weak bonding between the matrix and the fiber by spring element. In overall analysis, they have described the nonlinear behaviour of the composite and also their failure mechanism. Spanos et al.[13] have estimated the elastic mechanical properties of graphene-reinforced nanocomposites with the help of micromechanical finite element approach. In such analysis, C–C bond in graphene have been modeled using different nonlinear bond potential functions [15].

Tang et al. [16] have performed systematic molecular dynamic (MD) simulations to investigate the influence of silicon thickness and temperature on fracture characteristics of a graphene-silicon nanocomposite. Under different tensile loading, they found that the crack starts in silicon. Moreover, they have also mentioned that the size effect becomes insignificant if the film thickness is more than 20 Å. To explore the influence of graphene coated sheet on another substrate, Le and Umeno [17] investigated the fracture toughness of boronitrene(B-N), graphene (Gr) and their composites using molecular dynamics simulation. They found that the graphene with zigzag/armchair configuration has maximum fracture toughness. Consequently, they found that any initial crack developed in B-N and Gr composites unable to penetrate into graphene. Thus, it propagates in B-N region or along the interface of B-N and Gr composites. Jing and Aluru [10] have used molecular dynamics simulation for studying the mechanical properties of silicon nanofilm covered with graphene and have later extended their model [11] for including the effects of monoatomic vacancies and Stone-Wales defects of graphene. They have also investigated the fracture process of the silicon structure covered with graphene. Although, MD simulations is useful in accurately find the effects at atomic level in several cases, because of the restriction in time span and length scales it turns out to be less efficient in exploring the characteristics of mesoscale structures involving a huge number of atoms, molecules and chemical bonds. Therefore, an effort towards developing equivalent FEM approach has been put in by several researchers so as to reduce the computational time. However, it has certain limitations in capturing size/non-local effects. Tserpes et al. [18] have proposed an atomistic-based progressive fracture model for simulating the mechanical performance of carbon nanotubes (CNTs) using FEM. They have found that the fracture evolution, failure stresses and failure strains of nanotubes show similar results as obtained using other molecular mechanics approach. Xiao et al. [19] have developed an atomistic-based finite element model for predicting the fracture and progressive failure of graphene sheets and CNTs by incorporating the modified Morse potential. Papanikos et al. [20] have developed a 3D fatigue progressive damage model which integrates stress analysis, fatigue failure analysis and fatigue material property degradation (gradual and sudden) for carbon fibre-reinforced plastics laminates using 3D FEM in the ANSYS. They have performed fatigue failure analysis using a set of Hashin-type failure criteria and the Ye-delamination criterion. In this work, we have applied the progressive damage model of Tserpes [18] to study the fracture behaviour of GSNC. Thus, in this work, we have incorporated FEM-based model for GSNCs to obtain their mechanical behaviour and validate the results with the MD simulation results available in the literature.

There have been many studies related with the development of nonlinear atomistic finite element model, but most of them are limited to the analysis of single/multi-walled carbon nanotube or isolated graphene [21–26]. Here, we have applied molecular-structural mechanics based non-linear finite element analysis to study the mechanical properties of GSNC. In the proposed method, C–C bond in graphene is modelled with beam element and the modified Morse potential is used for simulating the elastic properties of isolated graphene. The silicon nanosheet is modelled as a continuum isotropic elastic medium by an appropriate shell element for simplicity. However, it could have been modelled as discrete structure depending on its molecular structure, but such approach would have significantly enhanced the computational cost and complexity of the whole model. The load transfer conditions between graphene and silicon nanosheet are modelled using bonded contact [27,28] connecting the two overlapping layers to simulate the interfacial region. The interface model considers perfect bonding between SLG and silicon nanosheet till the final failure. Hence, following the above procedure for SLG with either one (Gr-Si) or both sides (Gr-Si-Gr) of a silicon nanosheet, the interface between SLG and silicon is simulated using contact elements. This interfacial model is capable enough to simulate a wide range of interactions between graphene and silicon nanosheet. The nonlinear finite element modelling based on above approach is performed in ANSYS [29] to compute stress-strain curve under tensile loading and the fracture characteristics of SLG, silicon nanosheet and combined structures. The stress-strain curves obtained using FEM are compared with the MD simulation results [10] for different thicknesses of silicon nanosheet (Si) covered with SLG on one side (Gr-Si) as well as on both sides (Gr-Si-Gr) of silicon nanosheet, respectively. Subsequently, we have also analysed the mechanical properties of GSNC composites for three main orientations ⟨100⟩, ⟨110⟩ and ⟨111⟩ of silicon nanosheets and the effect of their varying thickness. Based on the analysis, we have found that the developed molecular-structural mechanics based FEM model can be used effectively to capture the elastic as well as fracture properties of GSNC as long as the size/non-local effects are neglected.

2. Molecular dynamics vs. finite element method

Molecular dynamics simulations impart in-depth information on molecular fluctuations and structural alterations and are used to analyse the thermodynamics and structure of biological and chemical molecules. Selection of accurate numerical algorithms and force field suited for MD simulations is crucial work. Very small time steps of the order of a femtosecond (10^{-15}) are generally used in MD due to very rapid oscillatory motions in the molecular system, so to get the desired parameter from simulation, requires a very long integration time. Although MD simulations provide explicit results in several cases, it has a restriction in the selection of time span and the length scales of the model. Thus, its application in exploring the characteristics of large structures involving a huge number of atoms, molecules and chemical bonds are limited [21,26,30].

To improve the modelling of graphene and CNTs, studies based on atomistic model as well as continuum model are essential. While molecular dynamic simulation study helps to accurately predict the phenomena at the atomic or molecular scale, equivalent continuum models are required to shorten the computational time without losing significant effects at that scale. Since, finding correct equivalent continuum model is based on the consideration of intra- and interatomic potentials associated with different degrees of freedom. Therefore, finite element method analysis based on beam elements which considers potential associated with C–C bond is valid under the condition when the potential associated with bending is negligible as compared to that due to stretching. Moreover, FEM based simulation may fail to capture accurate result if the size of graphene or CNTs is comparable to the bond length which is the biggest limitation of finite element based approach in simulating graphene and CNT based study. These two limitations are found to be negligible in the present case study presented in the paper.

Thus, we incorporate FEM based modelling for analyzing the elastic and fracture characteristics of graphene-silicon nanocomposites for different orientations and thicknesses of silicon as well as different configurations of graphene. The total run time for each of the FEM simu-