Mechanical simulation of a single sheet of graphene: a study on the applications of nanomaterials

Ricardo Silva Rosa Pedrosa
ricardopedrosa@ist.utl.pt

Instituto Superior Técnico, Lisboa, Portugal

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Abstract

Graphene is a bidimensional carbon allotrope with a hexagonal molecular lattice, in which its mechanical, electrical and optical properties have motivated an intense level of research of the scientific community in the last decade. This dissertation’s main objectives are the development of a consistent finite element model for the both linear and non linear simulation of graphene’s mechanical behaviour. Two interatomic potentials were used in the linear simulations of the model to assess their influence on the elastic properties. Non linear simulations were performed to obtain graphene’s mechanical strength. The finite element model results are compared with results collected from previous works on the fields of molecular dynamics and other atomistic computational methods. The present study shows that finite element models are able to predict well the mechanical properties of graphene.

Keywords: Graphene, Nanomaterials, Mechanical Properties, Interatomic Potential, Finite Element Method

1. Introduction

Nanostructured materials have attracted a considerable amount of interest and research in the last few years due to their remarkable mechanical, electrical and optical properties. In particular, graphene has been intensely studied, due its many applications. Some of the more applications are: structural composites like ceramic-graphene-ceramic ones that improve brittle fracture behaviour of the ceramics used in jet engines without compromising heat resistance, metal and polymer nanocomposites that are stiffer, stronger and lighter than most of the composites available today; in electronics, graphene and CNTs have been researched for future transistors that may greatly increase information processing speed; graphene is expected to improve hydrogen storage capabilities, and even efficient electrical power storage in the form of supercapacitors.

Graphene is a single graphitic layer of an hexagonal mesh of sp2 hybridized carbon-carbon bonds, in which its geometry is shown in figure. As so, its thickness isn’t defined, but its estimated as 3.4Å, the interlayer adhesion distance between layers in graphite. Even though, Lee obtained experimentally a Young modulus of 1 TPa and a strength of 130 GPa for graphene, by using an atomic force microscope. Multiple efforts have been made in order to predict graphene’s mechanical properties. Tsai used molecular dynamics simulations on graphene to obtain a Young modulus of 0.912 TPa, a Poisson coefficient of 0.26, and a shear modulus of 0.358 TPa. Liu used ab initio calculations using DFTP (a perturbation based variation of Density Functional Theory) to achieve a Young modulus of 1.05 TPa and a strength of 110-121 GPa for a fracture strain of 0.19-0.266. Still, these analysis methods require a great amount of computational effort and time investment, so it is presented, in this article, a methodology based in the Finite El-
ment Method (FEM), available and widely used in engineering applications, to study with precision and quickness the mechanical properties (linear elastic and non-linear) of graphene. Some authors have already used this method (originally devised by Odegard \[12\] with success: Meo and Rossi \[12\] used non linear springs to modulate the carbon links in CNTs and graphene, and obtained, for the last, a Young modulus of 0.945 GPa.

2. Background
2.1. Molecular mechanics

An important component in molecular mechanics calculations is the description of the forces between individual atoms. This description is characterized by a force field. In the most general form, the total inter-atomic potential energy in a molecule, \( U_{\text{total}} \), for a nano-structured material is described by the sum of many individual energy contributions related to the interactions between linked atoms, and non linked atoms, in the molecular lattice, as shown in the equation 1:

\[
U_{\text{total}} = \sum U_r + \sum U_\theta + \sum U_\omega + \sum U_{\text{vw}}
\]

In which the first four terms represent the interactions between bonded atoms and the fifth term, \( U_{\text{vw}} \) represents the van der Waals interaction between any non bonded atoms, often described by the Lennard-Jones potential \[3\], but here is despised due to its weak influence on the mechanical properties of graphene. The electrostatic term of the potential is also despised. The first four terms describe the atoms motion and position lattice. \( U_r \) is related to the axial deformation on the molecular link, \( U_\theta \) is the 'bending' term and it describes angular motion between three atoms and finally, \( U_\omega \) and \( U_{\text{vw}} \) are the in-plane and out-of-plane torsion terms. These interactions are easily interpreted from a basic molecule scheme depicted in figure 2.

![Molecule Scheme](image)

Figure 2: Geometry of a simple molecule chain where \( r_{23} \) is the interatomic distance, \( \theta_{234} \) is the 'bending' angle and \( \phi_{1234} \) the in-plane torsion angle \[3\].

Obtaining accurate parameters for a force field amounts to fitting a set of experimental or empirical data to the assumed functional form, specifically, the force constants and equilibrium structure of the molecule. In this article the AMBER \[2\] and Morse \[13\] interatomic potentials are used. They are both represented in their harmonized form in equation 2:

\[
U_r = \frac{1}{2} k_r (\delta r)^2,
\]

\[
U_\theta = \frac{1}{2} k_\theta (\delta \theta)^2,
\]

\[
U_\omega = \frac{1}{2} k_\omega (\delta \phi)^2.
\]

where \( k_r \) is the bond stretching force constant, \( k_\theta \) is the bond bending force constant and \( k_\omega \) is the equivalent bond torsion term, and \( \delta r \), \( \delta \theta \) and \( \delta \phi \) are the bond stretching increment, bond angle variation and angle variation of bond twisting, respectively.

2.2. Equivalent beam model

In order to determine the elastic moduli of the beam elements that will compose graphene’s structure, relations between the sectional stiffness parameters in structural mechanics and the force-field constants in molecular mechanics need to be obtained. For simplicity reasons, the sections of the bonds are assumed to be identical and circular. The elastic properties that need to be obtained are Youngs modulus \( E \), Poisson’s ratio \( \nu \) and the shear modulus \( G \). The deformation of a space-frame results in changes of strain energies. Thus, the elastic moduli can be determined through the equivalence of the energies due to the interatomic interactions presented in equation 2 and the elastic energy that results from the deformation of the space-frame structural elements. As each of the energy terms of equations 2 represents deformations in specific degrees of freedom, the strain energies of structural elements under the same deformations in equivalent degrees of freedom will be considered. According to the Euler-Bernoulli beam model from classical structural mechanics, the strain energy \( U_A \) of a uniform beam of length \( L \) and cross-section \( A \) under pure axial force \( N \) is:

\[
U_A = \frac{1}{2} \int_0^L N^2 \frac{E A}{E A} dx = \frac{1}{2} \frac{E A}{L} (\delta L)^2
\]

The strain energy \( U_M \) of a uniform beam with a moment of inertia \( I \), under pure bending moment \( M \) is:

\[
U_M = \frac{1}{2} \int_0^L M^2 \frac{E I}{E I} dx = \frac{1}{2} \frac{E I}{L} (2\alpha)^2.
\]

where \( \alpha \) denotes the rotational angle at the ends of the beam. The strain energy \( U_T \) of a uniform beam
under pure torsion $T$ is:

$$ U_T = \frac{1}{2} \int_0^L T^2 \frac{d\gamma}{J} \, dx = \frac{1}{2} \frac{GJ}{L} (\delta \beta)'^2. $$  

(5)

where $\delta \beta$ is the relative rotation between the ends of the beam and $J$ the polar moment of inertia.

The equivalence of bond stretch equation 25 and axial beam equation 27, bond and beam bending equations 28 29 and bond and beam torsion equations 30 31 serves as foundation of the equivalent atomic-beam model that is used in the analysis of graphene’s linear mechanical behaviour. This equivalence is presented in a more compact in the following equations:

$$\frac{EA}{L} = k_r, \quad \frac{EI}{L} = k_\theta, \quad GJ = k_T. \quad (6)$$

The thickness of a single sheet of graphene is not well defined, but for calculation purposes it has been estimated as 3.4 Å. As the length of the same carbon bond is estimated as 1.42 Å, the beam element that models this covalent bond will have a short aspect ratio, and therefore, the Timoshenko shear correction 32 can be introduced in the classical beam model of equation 33. This correction changes the bending energy equation to the form:

$$ U_{Timoshenko} = \frac{1}{2} \frac{EI}{L} (3 + \frac{1}{2} \Phi) (2\alpha)^2. \quad (7)$$

where $\Phi$ is the shear tension coefficient, represented by:given by the expression:

$$\Phi = \frac{12EI}{GA_\theta L^2}. \quad (8)$$

where $A_\theta = A/F_\theta$, $e F_\theta$ is the shear correction factor, which takes the following form for a circular section:

$$F_\theta = \frac{6 + 12\nu + 6\nu^2}{7 + 12\nu + 4\nu^2}. \quad (9)$$

The system of equations 34 establishes the foundation for the application of the theory of structural mechanics in modeling of graphene or other similar fullerene structures, for linear elastic simulation. For the non linear behaviour a more direct approach based on the Morse potential is used. This potential is described approximately by the force field of the equation:

$$ F = 2\beta D_c (1 - \exp^{-\beta r}) \exp^{-\beta r}. \quad (10)$$

where $\beta = 2.625 \text{Å}^{-1}$ is a constant that controls the ‘width’ of the potential, $D_c = 6.03105 nN \text{Å}$ is the dissociation energy and $r$ is the length of the covalent bond taken as 1.42 Å. In order to get the non linear stress-strain curve for the C-C bond, equation 35 is divided by the section area of the carbon bond, which is not well defined because of the ill defined thickness of graphene, so therefore the section area is taken as unitary for the non linear studies.

3. Methodology

In this section the finite element model development methodology is described. In the first subsection the model’s geometry, material models and element type are depicted. In the second subsection, the analysis with each own boundary conditions are defined for linear elastic simulations. In the third subsection, the non linear analysis are defined, along with the modifications to the model that were needed to study this behaviour.

3.1. Reference model

A finite element model was built in the FEM software ABAQUS/CAE ®. As both linear and non linear simulations run on the same geometry, the model used for the linear elastic simulations is hereby defined as the Reference model, and every definition made in this subsection is relative to the reference model. In the following subsection, some modifications are made based on the reference model as a starting point.

First, the hexagonal geometry of graphene, shown in figure 3 was generated through a series of Python scripts. A toolkit named Sci-kit nano 13 was imported and then, the code uses a graphene generator class that is featured within the toolkit, organizing the importation of node coordinates and lines to the ABAQUS python developing environment, by a simple algorithm based on graph theory. The geometry of the sheet is approximately squared with an edge of 10 nm. The armchair chiral direction of the sheet is aligned with the X-axis and the zig-zag chiral direction is aligned with the Y-axis.

![Graphene single sheet](image)

Figure 3: Final geometry of the graphene single sheet, with a 10nm edge size.

The element B21, included in the ABAQUS ® element library was chosen to simulate the C-C bond. This element is a beam element that is ruled by the Timoshenko beam theory, defined in a bidimensional space, and has two nodes (uses linear inter-
that have 6 degrees of freedom: 3 translational and 3 rotational, in every cartesian direction.

Regarding the material model, there will be four material models to be tested within the same framework of analysis. Two of the material models will be based on the Euler-Bernoulli beam approach of equation 1, one using AMBER force field and the other using the linearized Morse force field. The other two are developed using AMBER and Morse force fields, but now with the Timoshenko correction. The material model inputs (Young moduli and shear moduli, the Poisson coefficient of the C-C bond is taken as 0) are expressed in table 1, with the four beam model/potential combinations that were implemented on the software. The element section as taken as circular.

Table 1: Force field constants \( k \) derived from both interatomic potentials used and the results from equation 1 for \( E, G \) and section diameter

<table>
<thead>
<tr>
<th>Interatomic force fields</th>
<th>Data</th>
<th>AMBER</th>
<th>MORSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k ) ( \frac{nN}{A} )</td>
<td>( \frac{nN}{rad} )</td>
<td>( \frac{nN}{A} )</td>
<td>( \frac{nN}{rad} )</td>
</tr>
<tr>
<td>( k_y ) ( \frac{nN}{A} )</td>
<td>( \frac{nN}{rad} )</td>
<td>65.20</td>
<td>84.70</td>
</tr>
<tr>
<td>( k_y ) ( \frac{nN}{A} )</td>
<td>( \frac{nN}{rad} )</td>
<td>8.76</td>
<td>9.00</td>
</tr>
<tr>
<td>( k_y ) ( \frac{nN}{A} )</td>
<td>( \frac{nN}{rad} )</td>
<td>2.78</td>
<td>2.78</td>
</tr>
</tbody>
</table>

| Timoshenko beam |
|-----------------|---|---|
| \( E \) \( \frac{nN}{A} \) | \( \frac{nN}{A} \) | 167.132 | 292.992 |
| \( G \) \( \frac{nN}{A} \) | \( \frac{nN}{A} \) | 80.828 | 147.191 |
| \( d \) \( \frac{rad}{A} \) | \( \frac{rad}{A} \) | 0.834 | 0.723 |

| Euler-Bernoulli beam |
|----------------------|---|---|
| \( E \) \( \frac{nN}{A} \) | \( \frac{nN}{A} \) | 54.836 | 90.075 |
| \( G \) \( \frac{nN}{A} \) | \( \frac{nN}{A} \) | 8.7012221 | 13.912 |
| \( d \) \( \frac{rad}{A} \) | \( \frac{rad}{A} \) | 1.466 | 1.304 |

These four material models, with its respective section geometry, are now defined, so it is now possible to present the four simulations that were made in order to simulate the elastic behaviour of graphene for small deformations. Each simulation was tested with each combination of beam model/potential so a total of 16 simulations were conducted. The four simulations are:

- Uniaxial traction test in the armchair direction \((Ox)\) axis, in order to obtain \( E_x \) and \( \nu_x \).
- Uniaxial traction test in the zig-zag direction \((Oy)\) axis, in order to obtain \( E_y \) and \( \nu_y \).
- Biaxial traction test \((XY)\) plane, in order to obtain the bulk moduli \( K \) (in this case an area moduli).
- Shear test \((XY)\) plane, in order to obtain the shear moduli \( G \).

For the uniaxial tests, one edge was simply supported, constraining only the translational degree of freedom in the direction of the test, while on the other edge was applied a unitary displacement of 1 Å. On the biaxial test the center point of the sheet was constrained in every degree of freedom and the same unitary displacement was applied to every edge. Relative to the shear test, the center point was also constrained, and in every edge was applied a shear load, parallel to the edge direction, in order to apply two cancelling moments.

3.2. Non linear model

Regarding the non linear model, some modifications were made to the reference model, concerning the study of graphene non linear behaviour in order to obtain the mechanical strength of this nanomaterial. The geometry of this model wasn’t modified because it is the same material, therefore the same molecular geometry. To describe the mechanical behaviour of the C-C bond, the equivalent atomic-beam method is still used but the equivalence between structural and molecular mechanics is made directly thought the Morse potential in its non harmonized form of equation 11, as detailed in the previous section. This equation only expresses the stretching interaction, as in this section, the remaining interactions are despised.

The FEM software only works with true stress-strain, so the engineering stress that derives from expression 11 needs to be rewritten in its true form. Various interpolation points are defined within the true stress-strain curve, and then these points are fed as input to ABAQUS within two material models: an elastic one, in which a Young’s modulus of 33.6 nN/Å is defined as the slope of the linear section of the curve (with \( \nu = 0 \) as in the reference model) and a perfectly plastic one, to model the non linear behaviour of the C-C, in which a set of points relative to the plastic stress-strain pairs are given as input. Figure 12 shows the engineering, true and plastic stress-strain curves used in the non linear tests.

The last alteration made to the reference model is regarding the beam element, where in the non linear analysis it is used an hybrid two-node beam element, B21H, because in this analysis, large deformations are expected, and hybrid elements deal better with this specification, since both load and displacement are primary variables in the element definition.
The tests made to the non linear model, were the three tractions tests and the shear test described in subsection 3.1 with the same boundary conditions, plus two uniaxial tests in the armchair and zig-zag directions, that share all the boundary conditions with the previous uniaxial tests, but with a fully constrained edge, instead of a simply supported edge, to access the influence of a non uniform state of stress on the mechanical behaviour of graphene.

4. Results
   4.1. Linear results

As discussed previously in section 3, in order to achieve the linear elastic properties $E_i$, $\nu_{ij}$, $K$ and $G$, of a single sheet of graphene modelled in ABAQUS\textsuperscript{®}, four mechanical tests were simulated, two uniaxial tests in the armchair and zig-zag directions, a biaxial test and a shear test, with the deformed geometry for each test shown in figures 5-8.

In the uniaxial tests, a displacement of 1 Å was applied to one end of the sheet and the reactions were measured on the opposing end, which was simply constrained in the direction of the test. In the biaxial test, the variation of area and the reactions on the displaced edges were measured. Finally for the shear test, the same unitary displacements were
applied but in the direction parallel to the edges, instead of being applied on the normal direction of the edge. By measuring the reactions and the displacements, its simple to obtain the stress and strain values and the elastic properties, using basic relations from continuum mechanics expressed in the equations \( 11 \) to \( 13 \). For the uniaxial tests:

\[
E = \frac{\sigma}{\epsilon} , \quad \epsilon = \frac{u}{H}, \quad \sigma = \frac{\sum R}{H} \quad (11)
\]

where \( E \) is the Young moduli for the direction of the test, \( \sigma \) is the normal stress, \( \epsilon \) is the strain, \( u \) is the applied displacement, \( H \) is the edge size of the sheet of 10 nm, and \( R \) the nodal reactions. The Poisson’s ratio was calculated by dividing the transverse strain with the normal strain \( \epsilon \). For the biaxial test:

\[
K = \frac{\Theta}{2A}, \quad \Delta = \frac{\Delta A}{A_0}, \quad \Theta = \frac{\sigma_x + \sigma_y}{2} \quad (12)
\]

where \( K \) is the bulk moduli, that in the case of graphene is a bidimensional moduli. \( \Theta \) represents the directional average stress, \( \Delta \) is the relative area variation, which is the the deformed area minus the initial area divided by the last. Finally for the shear test:

\[
G = \frac{\tau}{\gamma}, \quad \tau = \frac{\sum R_x}{H}, \quad \gamma = \gamma_I + \gamma_{II} \quad (13)
\]

where \( G \) is the shear moduli, \( \tau \) is the shear stress, \( \gamma \) is the distortion angle which is the sum of the distortion angles on two opposite corners of the sheet.

Using the equations \( 11-13 \), the first objective of defining the linear elastic properties of graphene was achieved. But before that, by the inspection of the same equations, it is noticeable that the stress is 2D, because the sum of the loads is divided by a length and not by the section area. It is also known that this nanomaterial is bidimensional and that its thickness isn’t defined, but as its mechanical behaviour resembles the one observed in plates and shells, the interlayer distance between graphitic layers of 3.4 Ås used as graphene thickness \( 10 \) in order to obtain equivalent 3D moduli. Therefore the results from the various analysis with different interatomic potentials and beam models are presented in table 2 (in this table AMB relates to the AMBER potential and MOR to the linearized Morse potential). In table \( 3 \) comparison between the best results obtained in the present study (it will be discussed why the results presented are the best) and results from various studies (MD, DFT, FEM, Monte Carlo etc.) presented in the literature.

The observation of the results presented in table 4 shows that graphene has a slightly orthotropic behaviour, as the Young’s moduli in the armchair and zig-zag directions isn’t equal, nor is the Poisson’s ratio, but as the difference is so narrow (2% - 4%) graphene can be easily accounted as an isotropic material. The results from both interatomic potentials and both beam models also display that the stiffer direction is the zig-zag direction (aligned with the y axis) which contradicts the results in the literature \( 22 \). Regarding the Poisson’s ratio, a strange result appears using the euler-bernoulli model, in which for a material that is almost isotropic, the ratio is superior than 0.5. Using the Timoshenko beam theory the ratio decreases to 0.45-0.5 which is still a high transversal contraction rate. Therefore the Timoshenko beam theory presents the most convincing results, and also is the most correct form of modeling the covalent bond, due to the low aspect ratio of the bond being comparable to the aspect ratio of short beams. In a general way, the Timoshenko beam provides a more stiffer carbon bond model (even if the section area is smaller with this model, the increase in Young’s moduli is enough to increase the axial stiffness \( EA \)). Regarding the interatomic potential influence on the results, the Morse potential provides higher force-field constants \( k \), which ultimately leads to a stiffer structure. Ergo, the results used for comparison with the literature are the ones obtained with the Timoshenko beam and the Morse potential.

In table 3 are presented the results from the present work and the ones found in the literature, in order to validate the methodology applied in this study. The literature results come from similar methods that use the finite element method, from MD simulations, and from DFT and other statistical physics simulations like the Monte Carlo method \( 22 \). The results from MD and DFT theory are more accurate than the present ones, in principle due to the inclusion of quantic, thermodynamic and

<table>
<thead>
<tr>
<th>Property</th>
<th>Euler-Bernoulli</th>
<th>Timoshenko</th>
</tr>
</thead>
<tbody>
<tr>
<td>Armchair uniaxial test</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( E_x ) [TPa]</td>
<td>0.388</td>
<td>0.620</td>
</tr>
<tr>
<td>( \nu_x )</td>
<td>0.472</td>
<td>0.434</td>
</tr>
<tr>
<td>Zig-zag uniaxial test</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( E_y ) [TPa]</td>
<td>0.397</td>
<td>0.631</td>
</tr>
<tr>
<td>( \nu_y )</td>
<td>0.482</td>
<td>0.456</td>
</tr>
<tr>
<td>Biaxial test</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( K ) [TPa]</td>
<td>0.543</td>
<td>0.271</td>
</tr>
<tr>
<td>Shear test</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( G ) [TPa]</td>
<td>0.118</td>
<td>0.217</td>
</tr>
</tbody>
</table>

Table 2: Results from the linear analysis to the FEM model
many other parameters involved in the atomic scale. Some experimental studies are also presented, even if they don't provide the full spectrum of elastic properties, their results are the most accepted in the scientific community (mainly the results from Lee [11]).

By inspection of table 1 we can conclude that the results from the finite element method have a greater variability due to the different modeling procedures: Alzebdeh [4] used an equivalent continuum framework after using the atomistic-beam model and Reddy [?] minimized the potential energy of the beams to find the equilibrium structure of graphene and its stiffness. For the Young’s moduli, our results of 0.749-0.763 TPa for the armchair and zigzag directions respectively are closer to the ones obtained by Reddy with a difference of 11.8 % - 6.3 %, but with a not so satisfactory difference relative to the more accepted value of 1 TPa, found by Lee [11] and, in average, in many other MD studies. The results of the Poisson’s ratio are somewhat larger than the ones found in the MD and DFT studies. Regarding the bulk modulus, there are not so many results available, but our bulk modulus result is in the same scale with the one found in Zakharchenko [23] with a difference of 19.5 %. Our result of the shear modulus, is a lot smaller than the results obtained by MD and DFT, but is in agreement with the result of Scarpa [18] that used the same beam model applied in the present work.

4.2. Non linear results

The non linear test were made with the objective of defining the mechanical strength and make a fracture strain prevision of graphene, within the framework of FEM modelling. With this in mind, the same test that were set up in the linear tests were made, plus two more uniaxial tests in the armchair and zigzag direction with a fully constrained edge. These two additional test better simulate real applications (it is always harder to only constraint one degree of freedom, than simply constrain all motion in every direction) and will serve to infer where fracture behaviour may appear in the sheet’s structure.

The elastic results from the non linear model are presented in table 3, in conjunction with the elastic results from the linear analysis, in order to compare both linear and non linear models in their effectiveness in predicting elastic properties. In table 3, the strength and fracture strain results are shown. Results from the literature are also shown in both tables.

The non linear model provided higher values for the Young’s moduli of 0.904-0.924 TPa, which translates in an average increase of 20% in comparison to the linear model. These results are closer to the staple value of 1 TPa found in the experimental study of Lee [11] and, in average, in MD studies [22, 11], with an error in order of 10%. This increase arises because of the direct interpolation of the force-displacement relation of the Morse potential, instead of modelling the stiffness of the beam with the equivalence of the potential energies of a structural beam and a covalent bond. Regarding the biaxial test, the bulk modulus $K$ decreased 13.5 % in relation to the the linear model, result that is much closer to the ones found in the MD computational simulations [13], with a relative error of 3.4 %. The shear analysis also provided closer results of the shear modulus $G$ to the literature, with an error of 15.4%. In a general way, it can be concluded that the non linear model is a better approximation of the elastic behaviour of graphene than the linear model, due to the more direct approximation of the bond mechanical behaviour, which is validated by its results being closer to the ones found in the literature, in comparison with the linear results.

The non linear model was created not just as a better approximation for the elastic behaviour of graphene, but as a tool to obtain the strength $\sigma_f$ and the respective fracture strain $\epsilon_f$ of this nanomaterial, which demand a simulation of the response of the model’s structure to large displacements. With this in mind in table 3 are also shown the results for $\sigma_f$ and $\epsilon_f$ obtained through the uniaxial tests, $\sigma_f$ and $(\frac{\Delta A}{A})_f$ through the biaxial test and $\tau_f$ and $\gamma_f$ through the shear test.

Regarding the simply constrained uniaxial tests, the value of $\sigma_f$ obtained was 113.2 for the armchair direction, and 134.7 for the zig-zag direction, which present an error of 13.2 % in relation to the MD results [4] and 12.9 % in relation to the experimental results [11]. The $\epsilon_f$ result shows a relative deviation of 8.5 % in average for both directions, in relation to the experimental result of Lee [11].

There were found no relevant studies on the biaxial strength and fracture area variation of a single sheet of graphene. The most studied behaviour regarding shear strength of graphene, is the collapse of a multi sheet graphene structure due to interlayer shear loading. As to in-layer shear, the only relevant study was Min [13] that obtained a $\tau_f$ value of 97.15 GPa, which is 20.9 % greater then the value of 117.5 GPa obtained in the present work.

In regard to the influence of the full constraints applied on the two additional uniaxial tests, it is shown in figures 8 and 11 the plastic equivalent strain energy in the uniaxial tests in the armchair and zig-zag direction respectively. These figures provide a means to interpret how a graphene sheet would fracture when subjected to a axial load, being fully constrained on one edge.

By observing figure 11, it can be concluded that the fully constrain creates a curvature on the de-
Table 3: Comparison of the present work linear results and the ones in the literature.

<table>
<thead>
<tr>
<th>Author</th>
<th>$E_x$ [TPa]</th>
<th>$E_y$ [TPa]</th>
<th>$E$ [TPa]</th>
<th>$\nu_x$</th>
<th>$\nu_y$</th>
<th>$\nu$</th>
<th>$K$ ([N/m])</th>
<th>$G$ [TPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present</td>
<td>0.749</td>
<td>0.763</td>
<td>-</td>
<td>0.473</td>
<td>0.501</td>
<td>-</td>
<td>(239)</td>
<td>0.256</td>
</tr>
<tr>
<td>Alzebdeh [2]</td>
<td>0.990</td>
<td>0.100</td>
<td>-</td>
<td>0.109</td>
<td>0.110</td>
<td>-</td>
<td>-</td>
<td>0.455</td>
</tr>
<tr>
<td>Scarpa [18]</td>
<td>1.957</td>
<td>1.379</td>
<td>-</td>
<td>0.570</td>
<td>0.578</td>
<td>-</td>
<td>-</td>
<td>0.213</td>
</tr>
<tr>
<td>Reddy [?]</td>
<td>0.670</td>
<td>0.814</td>
<td>-</td>
<td>0.430</td>
<td>0.520</td>
<td>-</td>
<td>-</td>
<td>0.384</td>
</tr>
<tr>
<td>Huang [8]</td>
<td>-</td>
<td>2.690</td>
<td>-</td>
<td>-</td>
<td>0.412</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

(MD - molecular dynamics)

<table>
<thead>
<tr>
<th>Author</th>
<th>$E_x$ [TPa]</th>
<th>$E_y$ [TPa]</th>
<th>$E$ [TPa]</th>
<th>$\nu_x$</th>
<th>$\nu_y$</th>
<th>$\nu$</th>
<th>$K$ ([N/m])</th>
<th>$G$ [TPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tsai [22]</td>
<td>-</td>
<td>0.912</td>
<td>-</td>
<td>-</td>
<td>0.261</td>
<td>-</td>
<td>-</td>
<td>0.358</td>
</tr>
<tr>
<td>Ni [16]</td>
<td>1.050</td>
<td>1.130</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Min [14]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.450</td>
</tr>
</tbody>
</table>

(DFT and Monte Carlo)

<table>
<thead>
<tr>
<th>Author</th>
<th>$E_x$ [TPa]</th>
<th>$E_y$ [TPa]</th>
<th>$E$ [TPa]</th>
<th>$\nu_x$</th>
<th>$\nu_y$</th>
<th>$\nu$</th>
<th>$K$ ([N/m])</th>
<th>$G$ [TPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zakharchenko [23]</td>
<td>-</td>
<td>1.040</td>
<td>-</td>
<td>-</td>
<td>0.150</td>
<td>(200)</td>
<td>-</td>
<td>0.450</td>
</tr>
<tr>
<td>Zhao [?]</td>
<td>-</td>
<td>0.910</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Liu [11]</td>
<td>-</td>
<td>1.050</td>
<td>-</td>
<td>-</td>
<td>0.190</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

(Experimental)

<table>
<thead>
<tr>
<th>Analysis (properties)</th>
<th>Linear</th>
<th>Non linear</th>
<th>MD [22]</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>Armchair ($E_x$ [GPa], $\nu_x$)</td>
<td>749, 0.473</td>
<td>903.2, 0.128</td>
<td>1130, 0.261</td>
<td>1000</td>
</tr>
<tr>
<td>Zig-zag ($E_y$ [GPa], $\nu_y$)</td>
<td>763, 0.501</td>
<td>924.6, 0.148</td>
<td>1050, 0.261</td>
<td>1000</td>
</tr>
<tr>
<td>Biaxial ($K$ [GPa])</td>
<td>703</td>
<td>608</td>
<td>588</td>
<td>-</td>
</tr>
<tr>
<td>Shear ($G$ [GPa])</td>
<td>256</td>
<td>303</td>
<td>358</td>
<td>-</td>
</tr>
<tr>
<td>Armchair NUT ($E_x$ [GPa])</td>
<td>-</td>
<td>916</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Zig-zag NUT ($E_y$ [GPa])</td>
<td>-</td>
<td>937</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4: Elastic properties results from linear simulations and non linear, and literature results from MD simulations and experimental studies [10] (NUT stands for Non Uniform Tension)

<table>
<thead>
<tr>
<th>Analysis (properties)</th>
<th>Non linear</th>
<th>MD [22]</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>Armchair ($\sigma_{f_x}$ [GPa], $\epsilon_{f_x}$)</td>
<td>113.2, 0.229</td>
<td>120, 0.325</td>
<td>130, 0.25</td>
</tr>
<tr>
<td>Zig-zag ($\sigma_{f_y}$ [GPa], $\epsilon_{f_y}$)</td>
<td>134.7, 0.228</td>
<td>100, 0.439</td>
<td>130, 0.25</td>
</tr>
<tr>
<td>Biaxial ($\sigma_f$ [GPa], $\left(\frac{\Delta A}{A_0}\right)$)</td>
<td>112.2, 0.507</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Shear ($\tau_f$ [GPa], $\gamma_f$ [rad])</td>
<td>117.5, 0.487</td>
<td>97.150</td>
<td>-</td>
</tr>
<tr>
<td>Armchair TNU ($\sigma_{f_x}$ [GPa], $\epsilon_{f_x}$)</td>
<td>112.4, 0.218</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Zig-zag TNU ($\sigma_{f_y}$ [GPa], $\epsilon_{f_y}$)</td>
<td>134.8, 0.229</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 5: Results for the strength properties from non linear simulations, and literature results from MD simulations and experimental studies [10] (NUT represents Non Uniform Tension)

5. Conclusions

This article was a extended resume of the thesis that was set out to infer the linear and non linear formed shape of the structure, and it can be seen near the leftmost corners that there is a concentration in plastic strain energy in that area, which can be a zone prone to the start of fracture nucleation with this loading condition. In figure 10 this phenomena can be seen also near the upper right corner and lower left corner of the sheet, where this is a diffusion of plastic energy from the corner in direction to the center of the sheet, which may be a plausible fracture axis in this loading condition.
The mechanical properties of graphene with the development of a consistent FEM model. The methodology employed in the present work was proved to be a simple, fast and accessible method to the engineering industry to study and analyse the mechanical properties of graphene, and other nano-materials, without a relevant loss of precision. This is needed due to graphene many prospective applications in many fields, which will require a deep understanding of the mechanical behaviour of graphene, so it can be used in the advanced technological components of the future.

The main findings of this thesis can be summarized in brief: The atomic-beam equivalent model in conjunction with the finite element method were proven to be a useful methodology in the simulation of the mechanical behaviour of graphene. With low computational cost and processing, the results obtained for the mechanical properties of this nano-material had a satisfactory precision, in comparison with the results in the literature.

The influence of the interatomic potential of the C-C bond on the mechanical behaviour of the FEM model is relevant, so this choice must be analysed thoroughly in future works. The beam model approximation also generates a deviation in the results, so inspection of the aspect ratio of the nanostructure bond to analyse is also important (in the case of graphene, its bond aspect ratio demands the application of Timoshenko beam theory).

A non-linear model of the covalent bond with direct interpolation of the interatomic potential for the stiffness of the equivalent beam element, was proved to be a better method than the equivalence of potential energies of equation 6, in the characterization of graphene’s mechanical properties. This methodology provided an average Young modulus of 0.92 TPa which is in close to the value of 1 TPa obtained experimentally by Lee [10].

After the development of this thesis, it is believed that there are still many improvements to be done within the framework of the present work, as well as other future developments. These include:

- Use the FEM model in multi-physics analysis, in order to simulate the variation of the mechanical properties with temperature, or in the presence of electrical currents through the material.

- Parametrize the dimensions of the sheet, in order to infer the influence of its size in the obtained results.

- Create a nano-composite FEM model, which uses the sheet modelled in the present work as a reinforcement element in a dispersion of nano-platelets in a polymeric matrix, and conduct studies on the mechanical behaviour of said nano-composite.

Acknowledgements
I would like to thank my supervisor, Professor Nuno Silvestre, for giving me the unique opportunity to start what i think it is my life research objective, for all the technical support, and for the patience and guidance through all this process.

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My gratefulness goes in a great way to my all of my family and friends who helped me and guided me, and were always present in this path i took.

Finally, i would like to thank my girlfriend, Joana Baptista, for giving me strength, determination, belief and most importantly, love.
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