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Nanostructures Failures and Fully Atomistic Molecular Dynamics Simulations

José Moreira de Sousa

Abstract

Nowadays, the concern about the limitations of space and natural resources has driven the motivation for the development of increasingly smaller, more efficient, and energy-saving electromechanical devices. Since the revolution of "microchips", during the second half of the twentieth century, besides the production of micro-computers, it has been possible to develop new technologies in the areas of mechanization, transportation, telecommunications, among others. However, much room for significant improvements in factors as shorter computational processing time, lower energy consumption in the same kind of work, more efficiency in energy storage, more reliable sensors, and better miniaturization of electronic devices. In particular, nanotechnology based on carbon has received continuous attention in the world's scientific scenario. The riches found in different physical properties of the nanostructures as, carbon nanotubes (CNTs), graphene, and other exotic allotropic forms deriving from carbon. Thus, through classical molecular dynamics (CMD) methods with the use of reactive interatomic potentials reactive force field (ReaxFF), the scientific research conducted through this chapter aims to study the nanostructural, dynamic and elastic properties of nanostructured systems such as graphene single layer and conventional carbon nanotube (CNTs).

Keywords: molecular dynamics method, interatomic reactive force field—ReaxFF, graphene monolayer, convetional carbon nanotubes—(CNTs), elastic properties
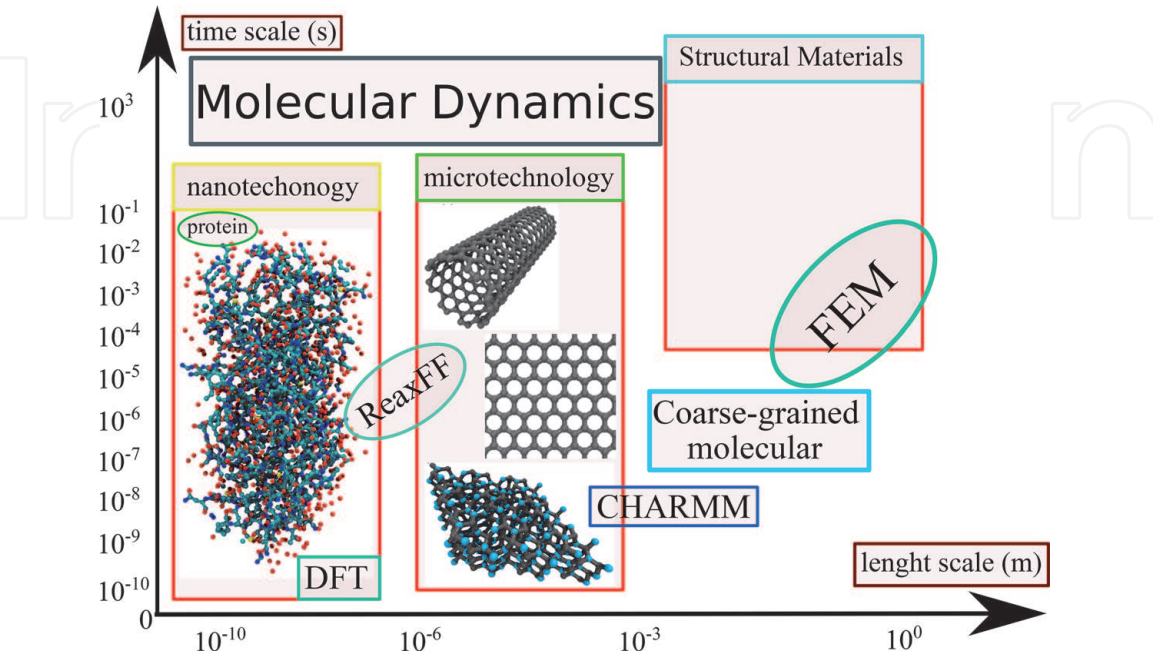
1. Introduction

Failures in condensed materials can be observed from the naked eye, Earth's crust in earthquakes, to the interatomic interaction of atoms and molecules at the nanoscale (nanoscience), not visible in experimental procedures that require explanations of certain physical phenomena on the nanometric scale [1].

Thus, understanding the condensed matter under mechanical load is of fundamental importance in the sustained development of new materials with superior qualities to the existing ones. Understanding the structural failure (even at the nanometric scale), the mechanical limits of new materials allow us to establish nanostructure applications and new materials for certain purposes the applicability in the development of new electromechanical devices to specific applicability's in advance nanotechnologies. Over several thousands of years, knowing the behavior of condensed matter under extreme conditions of mechanical stress has provided

the way for a new era in the science of materials and its modern technologies for improving the quality of life for humans and planet Earth. Due to nanotechnological advances, the human quality of life has important improvements in material science and its technologies. So, the basis of this advance is in the study of the physical properties of materials and nanostructures (theoretically as well as experimentally) and their various length and time scales for theoretical study for physicochemical predictions of nanostructures and materials. Fully atomistic molecular dynamics, like computational modeling, is becoming increasingly important and indispensable in theoretical description and predictions not understandable by experimental scientists in the development of new technologies [2, 3]. Nevertheless, starting to create nanostructures at the scale of atoms and molecules, atomistic models are described in terms of length-scale computational cost to obtain theoretical results of the physical properties of nanostructures and new materials. The following is an illustration of the computational cost of fully atomistic modeling at the scale of atoms and molecules [4], together with its computational methods widely used in computational modeling in materials science [5] (see **Figure 1**).

A fundamental and very important concept in the study and analysis of mechanical failure in nanostructures and new materials is to establish valid methods obtained from experimental averages. Thus, it is possible to establish a fully atomistic computational modeling to model the physical properties of nanostructures and new materials, where the set of parameters described in the reactive and non-reactive force fields are obtained directly from the results provided by the experiments. Currently, the combination of experimental tests with computational modeling concepts has shown promising and efficient results in the study of the physical properties of nanostructures and new materials at accessible computational cost scales with the dimensions of the nanostructure (number of atoms and molecules) [6, 7]. This strategy in nanotechnology has contributed to important results in simulations of atoms and molecules in scientific and technological innovation and applications [4, 8]. Thus, simulations with carbon nanostructures have received particular attention after the synthesis of graphene, which won a Nobel Prize for K.S. Novoselov, A.K. Geim in 2004 [9] (by mechanical exfoliation method of graphite), thus suggesting a new era in materials science and fully atomistic
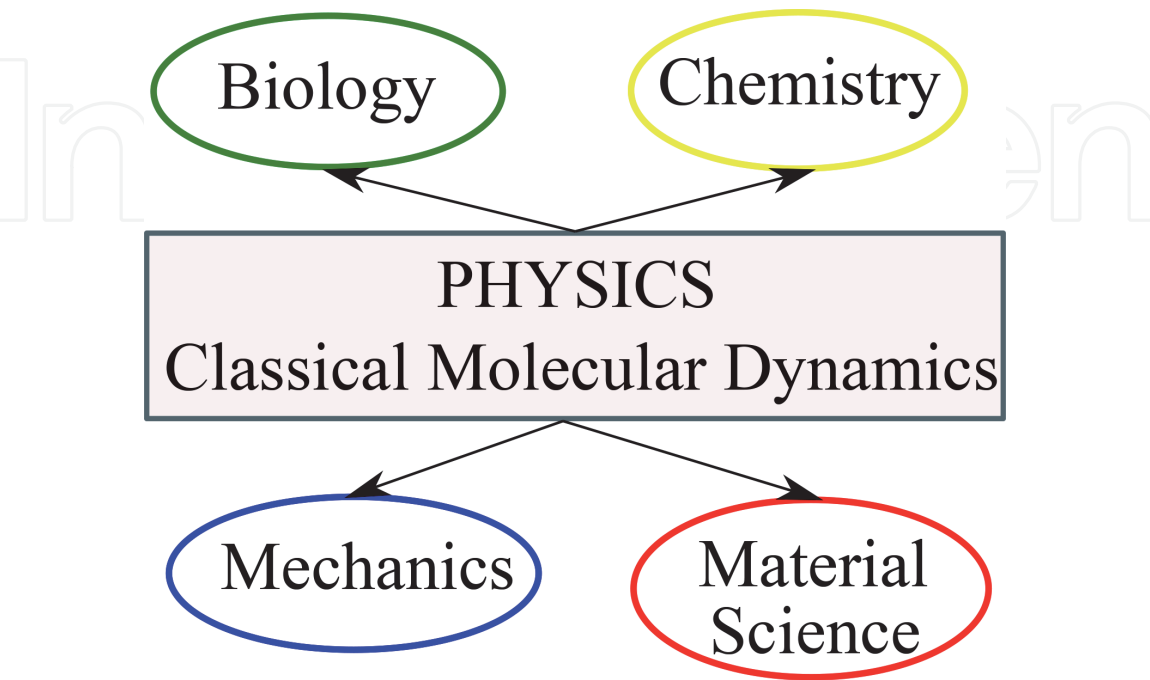

Figure 1.
Overview of a diagrammatic representation of timescales and lengthscale associated with computational methods used for computational simulation in the development of new materials in time and length scales [4].

computational simulations of systems formed by carbon atoms, particularly such as "graphene", a single layer of graphite and carbon nanotubes (CNTs), the cylindrical shape of roll-up one-dimensional graphene membrane (CNTs) [10].

In this chapter, we present the mechanical properties of graphene and CNT. We seek to show the efficiency of computational methods of reactive molecular dynamics with interatomic potentials parameterized by experimental results. We show theoretical results of mechanical failures in graphene monolayers and CNTs at the nanometer scale. Through computer simulations via classical molecular dynamics (CMD) method using the reactive force field (ReaxFF) reactive interatomic potential, we show mechanical failures (fracture pattern), Young's modulus, ultimate tensile strength (UTS), and critical strain for graphene and CNT and thus compare with the experimental results obtained in the literature. We hope that this chapter will add to future scientists who seek to start their academic activities using the molecular dynamics method with reactive potentials for studies not only of mechanical failures in nanostructures, but also more complete and detailed studies of the physical properties of nanostructured systems in nanometric scale.

2. Classical molecular dynamics simulation method

Classical molecular dynamics (CMD) is a technique that studies the behavior of a system of particles (atoms and molecules) as a function of time. The temporal evolution of set of these particles, in certain interacting systems, are obtained by the integration of equations of motion. Based on this, terms like "modeling" and "simulation" are widely used in conjunction with the numerical solution of physical problems involving interacting particles. However, it is important to note that these words have different meanings. The term "Modeling" refers to the development of the mathematical model of a physical situation, while "Simulation" refers to the procedure for solving equations, resulting in the developed model. This makes MD a widely used tool for studying material properties as an intersection of various scientific disciplines as shown in **Figure 2** [3].
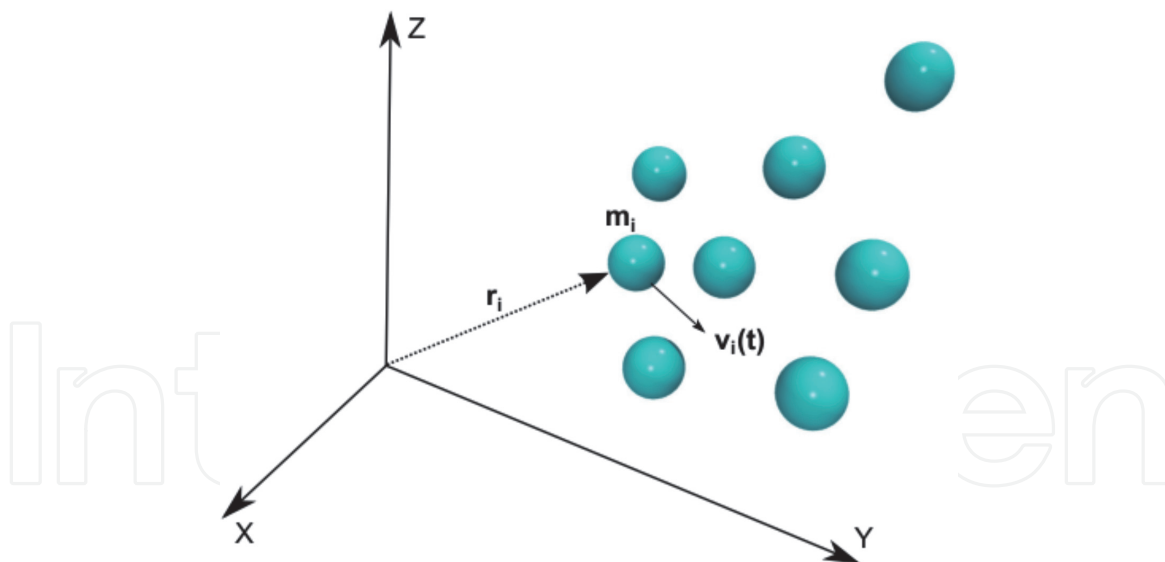

Figure 2.
Classical molecular dynamics method (CMD) as an intersection of several disciplines.

CMD simulations is a method that calculates the equilibrium and thermal transport properties in classical systems involving many bodies (in this case atoms as classical particles). In this context, the word "classic" means that the movement of these particles obeys the laws of classical mechanics (Newton's laws), being an excellent approximation for the study of the physical properties of a large number of nanostructures and new materials, especially graphene and CNT (in a study in this chapter). This method consists of solving Newton's equations for a set of atoms and molecules, thus obtaining the speed and position of each particle that makes up the physical system at each instant of the simulation. The theoretical basis of CMD embodies many of the results produced by great names in analytic mechanics such as: Euler, Hamilton, Lagrange, and Newton. Your contributions can be found in mechanics textbooks [11–13]. Some of these results contain fundamental observations of nature, while the others are elegant reformulations in the theoretical development of a classical mechanics set of linked computers that work together (computer cluster), perform computational calculations as a single system. The shared memory is performed by multi-threading parallelism (OpenMP) for computational clusters. Thus, after having the code installed and depending on what you want to simulate, it is necessary to build a computational code in C++ language, where we establish the physical properties of the problems to be studied by performing the computational modeling. For example, in this review chapter, we will simulate the mechanical failures of graphene and CNTs by the CMD-ReaxFF method. The code is written in computational language C++, where the thermodynamic quantities output via the "thermo-style" command is important to normalize all physics quantities by the number of atoms. This behavior can be changed via the thermo-modify (in real units) norm command. After the initial definitions of the code, we establish the statistical set that will describe the physical properties of the computational sample that we intend to computationally simulate, such as the NVT statistical canonical ensemble. In many cases, because the system has a very large number of particles, it is impossible to find the properties of such complex systems analytically. The trajectories of atoms and molecules are determined through from the numerical solution of Newton's equations of motion, to a system with interacting particles, where the force between the particles and the potential energy are defined by mechanics force field molecular (here reactive force field—ReaxFF discussed in following section).

Therefore, the objective in an atomistic simulation is to predict the movement of each atom in a material, characterized by a set of linked computers that work together (computer cluster), perform computational calculations as a single system. The shared memory is performed by multi-threading parallelism (OpenMP) for computational clusters. Thus, after having the code installed and depending on what you want to simulate, it is necessary to build a computational code in C++ language, where we establish the physical properties of the problems to be studied by performing the computational modeling. For example, in this review chapter, we will simulate the mechanical failures of graphene and CNTs by the CMD-ReaxFF method. The code is written in computational language C++, where the thermodynamic quantities output via the "thermo-style" command is important to normalize all physics quantities by the number of atoms. This behavior can be changed via the thermo-modify (in real units) norm command. After the initial definitions of the code, we establish the statistical set that will describe the physical properties of the computational sample that we intend to computationally simulate, such as the NVT statistical canonical ensemble: the atomic position $r_i(t)$, the velocities $v_i(t)$, and accelerations $a_i(t)$, as shown in **Figure 3.** The general idea of running a molecular dynamics simulation is presented by two factors as followed:

Figure 3.
Illustration of a system with N carbon atoms interacting with each other by interatomic reactive potentials, here in this chapter the ReaxFF reactive force field will be presented (see [4]).

1. Particle under the effect of potential energy, of where the forces governing the system can be calculated.

2. Equations of motion that determine the dynamics of particles, in which case Newton's laws are applied. Molecular dynamics uses Hamilton's classical equations of motion.

The classical Hamiltonian is defined as the sum of kinetic energy and energy potential:

$$p = -\frac{\partial H}{\partial R_i} \tag{1}$$

and

$$\dot{R} = -\frac{\partial H}{\partial p_i} \tag{2}$$

that lead to Newton's equations of motion. The classical Hamiltonian is defined as:

$$H(p_i, R_i) = \sum_{i=1}^{N} \frac{p_i^2}{2M_i} + V(R_i) \tag{3}$$

The force on an atom can be calculated by Newton's law as the derivative of energy in relation to the change in the position of the atom:

$$F_i = m_i \frac{d^2 Ri}{dt^2} = -\nabla_i V(R_i) = -\frac{dV}{dR_i} \tag{4}$$

leading to the set of Newtonian equations of motion for each particle i with mass m_i and Cartesian coordinate R_i. Therefore, for a closed system composed of N carbon atoms that interact through a potential energy function (here the interatomic reactive force field—ReaxFF), the CMD consists of solving the coupled N Newton equations. Therefore, in a computer simulation, we use a numerical integration algorithm to solve N differential equations [14].

In the classical formalism of CMD, the carbon atoms are treated as a collection of classical particles that can be described by Newtonian forces, where they are treated by harmonic or elastic forces. A complete set of interaction potentials between particles is known as the force field [15]. Parameters associated with force fields can be determined via first-principle calculations (Density Functional Theory—DFT) or via experimental results. Currently, there are numerous cam types of forces that are widely used in the study of the physical and chemical properties of nanostructured systems. We present in this chapter the interatomic force field—ReaxFF in the study of mechanical failure (mechanical properties) of a single layer of graphene and CNTs (armchair and zig-zag). In followed section, we show a brief description of the force field used in the simulations presented here in this chapter about the mechanical properties of graphene and CNT.

3. Interatomic reactive force field: ReaxFF

The reactive force field (ReaxFF) was developed to be a bridge between the chemical-quantum (QC) and the empirical (EFF) force fields [16, 17]. The EFF methods [18] describe the relationship between energy and geometry using a relatively simple set of functions. In the simplest form, EFF methods treat CMD systems or condensed matter systems by simple harmonic equations that describe the stretching and compression of bonds and the bending of bond angles. Unbound interactions are described by van der Waals potentials and Coulomb interactions (Lennard-Jones potential):

$$V_{LJ} = 4 \in \left[\left(\frac{x}{\sigma}\right)^{-12} - \left(\frac{x}{\sigma}\right)^{-6} \right] \tag{5}$$

The Lennard-Jones potential consists of a two-body interaction function composed of the sum of two terms, an attractive interaction of the van der Waals type $\approx 10^{-6}$ and a short-range repulsive interaction $\approx 10^{-12}$ associated with the repulsion between orbitals atomic due to the Pauli exclusion principle. The terms # is a measure of the depth of the potential well and the term σ is the coefficient of the expression of the equilibrium distance of the pair of atoms. Classic models are not the only possible way to develop the potentials of many bodies. Developments based on first principles can lead to more accurate potentials for describing cases of interest. In this class of more modern potentials are included the so-called reactive potentials, developed specifically for a description of the dynamics of formation and breaking of bonds in materials. As reactive potential, we have the ReaxFF [16, 17], potential using in the chapter in the description of the physical properties of failure mechanics of graphene single layer and CNT. The CMD-ReaxFF is performed in all calculations in this chapter in the review study of mechanical properties of graphene single layer and CNTs. We show the interesting and important method, because through the theoretical results the values obtained in all simulations are in good agreement with experimental results and with results based on quantum methods (ab initio and DFT).

The modern reactive force field (ReaxFF) is parametrized whit first-principles calculations and compared with experimental results. The heath formations of the carbonous nanostructures values change between 2.8 and 2.9 kcal/mol when compare reactive molecular dynamics simulations and data experimental [16, 17]. The set parameter validity used for performed reactivity between carbon atoms ligands in this reviewer is divided by partial energy contributions [16, 17]:

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{tor} + E_{conj} + EvdW + E_\infty, \quad (6)$$

where, here the terms of Eq. (6), respectively, represents the energies corresponding to the bond distance (E_{bond}), the over-coordination (E_{over}), the undercoordination (E_{under}), the valence (E_{val}), the penalty for handling atoms with two double bonds (E_{pen}), the torsion (E_{tor}), the conjugated bond energies (E_{conj}), the van der Waals ($EvdW$), and coulomb interactions (E_{co}). The fundametation of ReaxFF is bond order BO'_{ij} between a pair of atoms as [16, 17]:

$$BO'ij = \exp\left[pbo, 1. \left(\frac{r_{ij}}{r_o}\right)^{pbo,2}\right] + \exp\left[pbo, 3. \left(\frac{r_{ij}^\pi}{r_o}\right)^{pbo,4}\right] + \exp\left[pbo, 5. \left(\frac{r_{ij}^\pi}{r_o}\right)^{pbo,6}\right]$$
$$(7)$$

where the atomic configurations is obtained from interatomic distance r_{ij} of three exponential terms, such as, the σ bond ($pbo, 1$) and ($pbo, 2$), first π bond ($pbo, 3$) and ($pbo, 4$) and $\pi\pi$ bond ($pbo, 5$) and ($pbo, 6$), with their respective dependencies in interatomic distances C—C bond ($\sigma \sim 1.5A$), ($\pi \sim 1.2A$) and ($\pi\pi \sim 1.0A$).

The bond order is corrected for cases where there is over-coordination (more bonds than allowed), through f_1 and residual link order BO' for valence angles, through f_4 and f_5. The correction due to over-coordination occurs only for bonds between two carbon atoms, while the correction for the residual bond order BO' for valence angles occurs for all connections. The corrections f_i, ($f_i = 1...5$) are presented in Eqs. (11)–(15). Bond order BO' for valence angle refers to the bond order existing between two atoms, not directly connected, where both are connected to a third, forming a valence angle [16, 17]:

$$BO_{ij} = BO'_{ij}.f_1\left(\Delta'_i, \Delta'_j\right).f_4\left(\Delta'_i, BO'_{ij}\right).f_5\left(\Delta'_j, BO'_{ij}\right)$$
$$BO_{ij}^\sigma = BO_{ij}'^\sigma.f_1\left(\Delta'_i, \Delta'_j\right).f_4\left(\Delta'_i, BO'_{ij}\right).f_5\left(\Delta'_j, BO'_{ij}\right) \quad (8)$$
$$BO_{ij}^\pi = BO_{ij}'^\pi.f_1\left(\Delta'_i, \Delta'_j\right).f_1\left(\Delta'_i, \Delta'_j\right).f_4\left(\Delta'_i, BO'_{ij}\right).f_5\left(\Delta'_j, BO'_{ij}\right)$$

$$BO_{ij}^{\pi\pi} = BO_{ij}'^{\pi\pi}.f_1\left(\Delta'_i, \Delta'_j\right).f_1\left(\Delta'_i, \Delta'_j\right).f_4\left(\Delta'_j, BO'_{ij}\right).f_5\left(\Delta'_j, BO'_{ij}\right) \quad (9)$$

$$BO_{ij} = BO_{ij}^\sigma + BO_{ij}^\pi + BO_{ij}^{\pi\pi} \quad (10)$$

$$f_1\left(\Delta'_i\Delta'_j\right) = \frac{1}{2}\left(\frac{Val_i + f_2\left(\Delta'_i\Delta'_j\right)}{Val_i + f_2\left(\Delta'_i\Delta'_j\right) + f_3\left(\Delta'_i\Delta'_j\right)} + \frac{Val_i + f_2\left(\Delta'_i\Delta'_j\right)}{Val_i + f_2\left(\Delta'_i\Delta'_j\right) + f_3\left(\Delta'_i\Delta'_j\right)}\right)$$
$$(11)$$

$$f_2\left(\Delta'_i\Delta'_j\right) = \exp\left(\lambda_1\Delta'_j\right) + \exp\left(-\lambda_1\Delta'_j\right) \quad (12)$$

$$f_3\left(\Delta'_i\Delta'_j\right) = \frac{1'}{\lambda_2}\ln\left\{\frac{1}{2}\left[\exp\left(-\lambda_2\Delta'_i\right) + \exp\left(-\lambda_2\Delta'_j\right)\right]\right\} \quad (13)$$

$$f_4\left(\Delta'_iBO'_{ij}\right) = \frac{1}{1 + \exp\left[-\lambda_3.\left(\lambda_4BO'_{ij}BO'_{ij} - \Delta'_i\right) + \lambda_5\right]} \quad (14)$$

$$f_5\left(\Delta_i' BO_{ij}'\right) = \frac{1}{1 + \exp\left[-\lambda_3 \cdot \left(\lambda_4 BO_{ij}' BO_{ij}' - \Delta_i'\right) + \lambda_5\right]} \tag{15}$$

There are ReaxFF implementations, developed by individual research-based in [16, 17] formalism. Nowadays, the current ReaxFF parameter set developed by CMD-ReaxFF based on the periodic table of elements found on our planet Earth are [18, 19]:

- Group 1: H (non-metal), Li, Na, K, Rb, Cs (metals).

- Group 2: alkaline Earth metal: Mg, Ca, Sr and Ba.

- Group 3: lanthanide: Y.

- Group 4: lanthanide: Ti, Zr and Hf.

- Group 5: lanthanide: V and Nb.

- Group 6: lanthanide: Cr, Mo and W.

- Group 7: lanthanide: Mn.

- Group 8: lanthanide: Fe and Ru.

- Group 9: lanthanide: Co.

- Group 10: lanthanide: Ni, Pd and Pt.

- Group 11: lanthanide: Cu, Ag and Au.

- Group 12: lanthanide: Zn.

- Group 13: B, Al and Ga.

- Group 14: C and Si.

- Group 15: N and P.

- Group 16: O, S, Se and Te.

- Group 17: F, Cl and I.

- Group 18: He, Ne, Ar, Kr and Xe.

So, in this chapter, we performed reactive molecular dynamics simulations with ReaxFF to obtain the failure mechanics of a single layer of graphene and CNT. The results of reactive molecular dynamics simulations performed in this chapter (CMD-ReaxFF) of review are discussed in the next section.

4. Large-scale atomic/molecular massively parallel simulator code: LAMMPS

All simulations developed in this thesis were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) code [20]. LAMMPS is a

code that simulates a set of particles (solid, liquid or gas) using the classical molecular dynamics method. It is a code designed to obtain efficiency in the simulation when it is performed on parallel processors for systems whose particles are in a 3D rectangular box with density approximately uniform. It is an open source program maintained and distributed by researchers at Sandia National Laboratories [20], written in C++. It's a stable program that has the ability to simulate from a few particles to billions of them. In the following chapters we present the results that were obtained with the use with LAMMPS code.

4.1 Computational modeling of mechanical failure of nanostructures

LAMMPS code is a classical molecular dynamics simulation in language C++ designed to run efficiently on parallel computers. Is an open-source code, distributed freely under the terms of the GNU Public License (GPL) developed at Sandia National Laboratories [20]. The LAMMPS runs on a single processor or in parallel, or in single laptops or advanced computational clusters parallel using memory message-passing parallelism (MPI) [21].
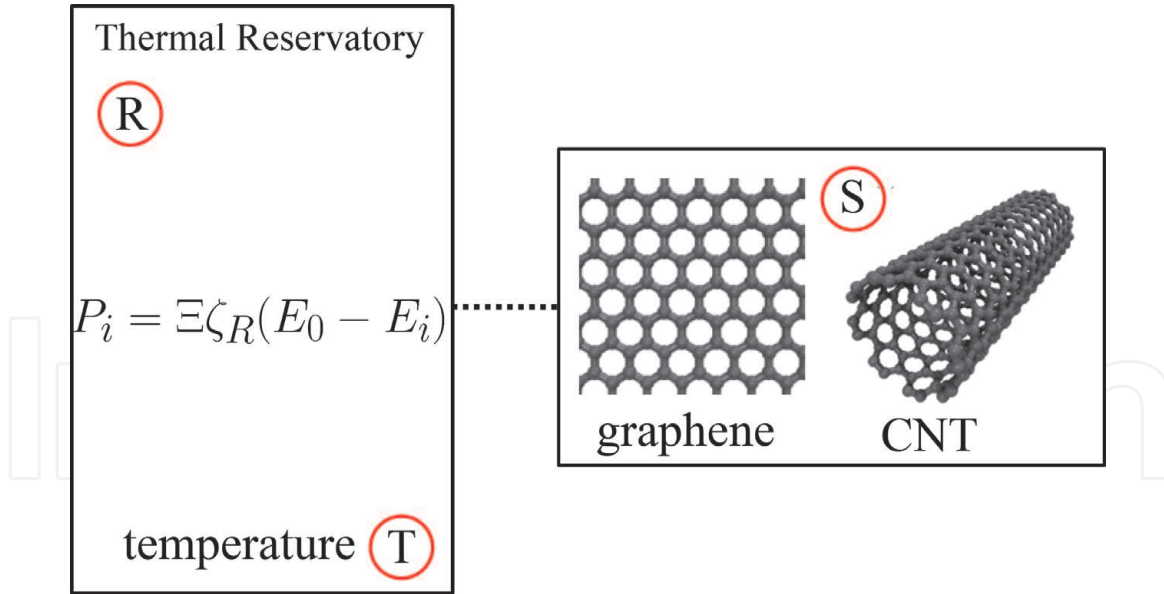
A set of linked computers that work together (computer cluster), perform computational calculations as a single system. The shared memory is performed by multi-threading parallelism (OpenMP) for computational clusters. Thus, after having the code installed and depending on what you want to simulate, it is necessary to build a computational code in C++ language, where we establish the physical properties of the problems to be studied by performing the computational modeling. For example, in this review chapter, we will simulate the mechanical failures of graphene and CNTs by the CMD-ReaxFF method. The code is written in computational language C++, where the thermodynamic quantities output via the "*thermo-style*" command is important to normalize all physics quantities by the number of atoms. This behavior can be changed via the thermo-modify (in real units) norm command. After the initial definitions of the code, we establish the statistical set that will describe the physical properties of the computational sample that we intend to computationally simulate, such as the NVT statistical canonical ensemble:

$$\text{fix ID group} - \text{ID nvt temp } T_{initial} \ T_{final} \ T_{damp} \tag{16}$$

After the initial definitions of the code, we establish the statistical set that will describe the physical properties of the computational sample that we intend to computationally simulate, such as the NVT statistical ensemble. The NVT commands perform time integration on Nose-Hoover thermostat [22] style designed to generate positions and velocities of computational sampled under computational modeling by CMD-ReaxFF.

5. Canonical ensemble in statistical mechanics and thermodynamics quantities

Characterized by a set of macroscopic parameters, graphene, and CNT are in contact with the thermal reservoir (see **Figure 4**). Considering the very large reservoir compared to the computational sample that we intend to study, the total energy of the E_0 system, we have the validity of the thermodynamic postulates and statistical mechanics. Thus, the probability Pi of obtaining physical quantities of interest, in these cases, in the study of the mechanical failure of graphene and CNTs is given by [23]:

Figure 4.
Computational sample (graphene and CNT) in contact with a thermal reservoir R *at a specific temperature different at 0.*

$$P_i = \Xi \zeta_R (E_0 - E_i) \tag{17}$$

where Ξ is a normalization constant, E_i is the energy of the system in the particular thermodynamics state i, and ζ_R is a microscopic state accessible to the thermal reservoir with energy E.

After coupled canonical thermostat NVT in the graphene and CNT, we applied a constant engineering strain rate of $\delta = 10^{-6}$ fs^{-1}, see de command line in LAMMPs code:
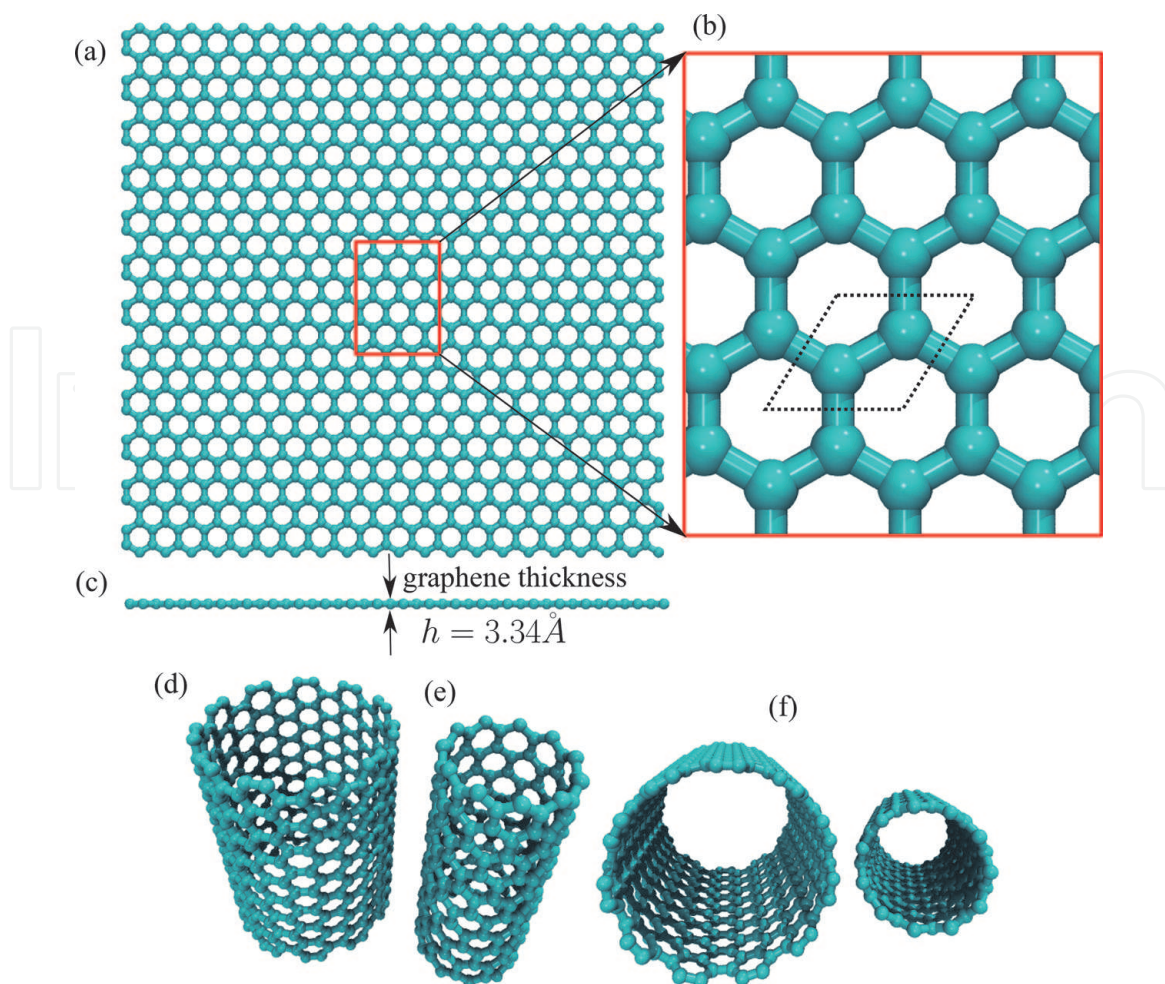
$$\text{fix ID group} - \text{ID deform N parameter args} \dots \text{keyword value} \dots \tag{18}$$

and so, adapt the code to the mechanical problem that seeks to study its elastic physical properties.

6. Fully atomistic computational simulation: elastic properties of graphene and CNT

After all the technical and physical properties in the study of mechanical failure in nanostructured systems, we present below the elastic properties of graphene single layer and CNTs (see **Figure 5**). In the **Figure 5**, we showed que atomistic configurations of graphene single layer $90 \times 90°$ A whith 3256 carbon atoms, conventional carbon nanotubes whthi chirality armchair (11, 11) whith 616 carbon atoms and zig-zag (11, 0) whith 352 carbon atoms.

Thus, in **Figure 6**, we can see the graphical representations of the stress/strain curve for graphene monolayer at 300, 600, and 1000 K temperatures. For graphene monolayer at 300, 600 and, 1000 K (black, red, and blue curves), we clearly note two regimes: first, a linear regime followed by a plastic regime up to the complete fracture (see **Figure 6**). At 300 K, our results obtained by fully-atomistic reactive molecular dynamics simulations performed with interatomic force field ReaxFF we can see at room temperature a linear regime, we do not see permanent deformations which are different from what occurs for the plastic regime, where the graphene monolayer present breaking bonds (aligned in directions of load strain applied) between carbon atoms C—C up to the fracture point, which is characterized by an
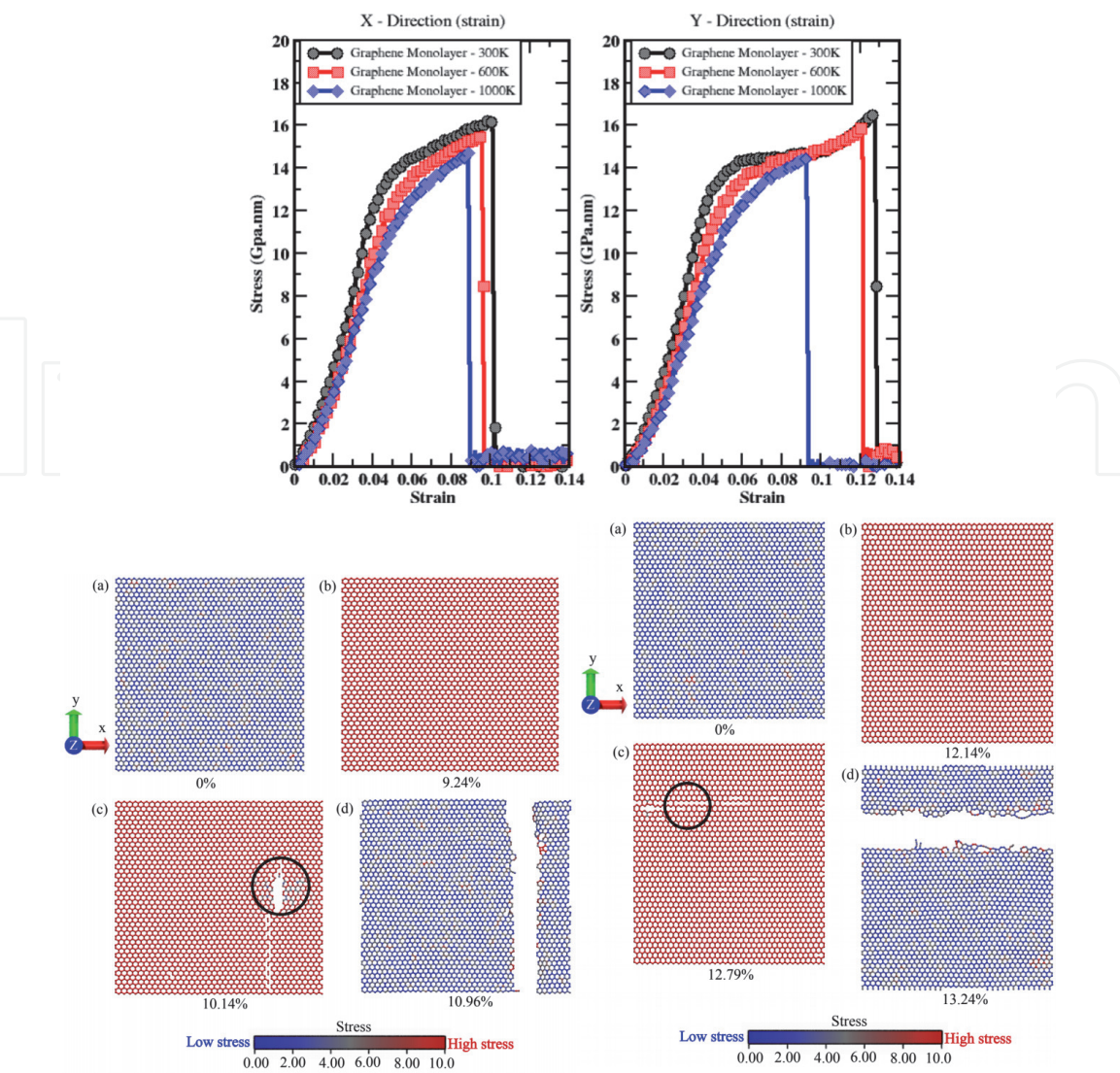
Figure 5.
Computational sample (graphene and CNT) in contact with a thermal reservoir R at a specific temperature different at 0.

abrupt drop of stress values to zero at 0.10 (0.13)—critical strain, respectively for X-direction (Y-direction). For higher temperatures (600 K and 1000 K), the stress/strain curves for graphene shows a reduction in ultimate tensile strength (UTS) and critical strain (σC) values. Those results for graphene were already observed for another theoretical investigation of graphene monolayer under thermal effects, see the bibliographic references [24, 25]. So, our results have good correspondence with results already obtained in the literature [26–28]. Therefore, the averages of the mechanical properties are listed in the following **Table 1**. In **Figures 6** and 7, we show the temporal atomistic evolutions of frames of the results obtained by reactive molecular dynamics simulations with an interatomic reactive force field ReaxFF, when the set of atomic configurations of load strain applied in graphene are in X and Y-direction and CNT.

In the results in **Figures 6** and 7, we can see the fully atomistic reactive molecular dynamics simulations with ReaxFF-potential for graphene monolayer for strain applied in X and Y-direction of mechanical load strain applied respectively. The results obtained whit ReaxFF potential show that the failure starts at C—C bonds which are aligned (in X and Y-direction of load strain applied). In all temperatures (300, 600, and 1000 K) we can see a clean failure rupture. The color bar in down of snapshot frames, shows the stress concentration in the monolayer the stretching dynamics, where the color blue are low-stress concentration and red color are high-stress concentrations in graphene monolayer. The results of CMD-ReaxFF for CNTs (armchair and zig-zag) (**Figure 7**), the stress is highly accumulated on the zigzag
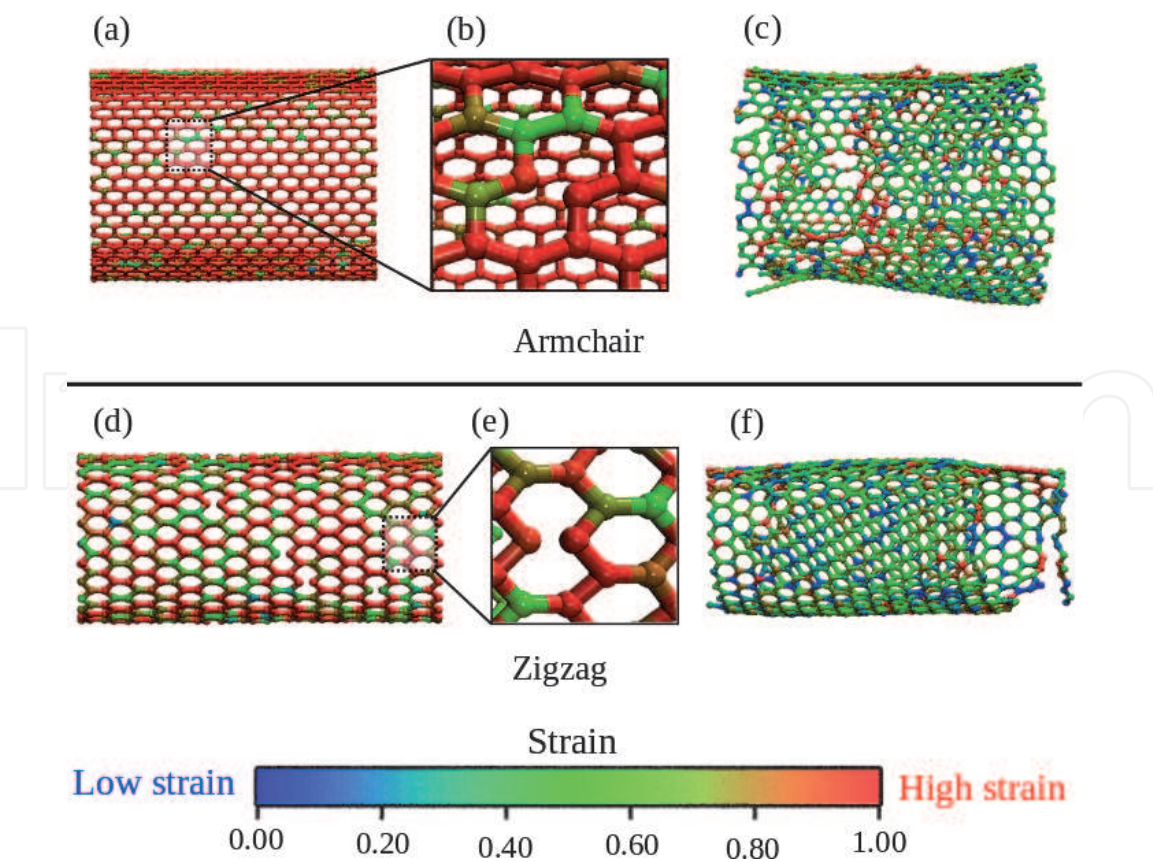
Figure 6.
Stress versus strain curves for graphene monolayers predicted by reactive molecular dynamics simulations with the ReaxFF interatomic potential at 300 K, 600 K and 1000 K in X-direction (left panels) and in Y-direction (right panels). Atomic frames representations of graphene monolayer under strain load in X-direction (room temperature): left side: (a) stretched (0%) of strain, in (b) 9.24% of strain, in (c) start break some chemical bonds C—C at 10.14% of strain and (d) the complete fracture of graphene monolayer at 10.96% of strain. In right side: atomic frames representations of graphene monolayer under load strain in Y-direction (room temperature): (a) un stretched (0%) of strain, in (b) 12.14% of strain, in (c) start break some chemical bonds C—C at 12.79% of strain and (d) the complete fracture of graphene monolayer at 13.24% of strain.
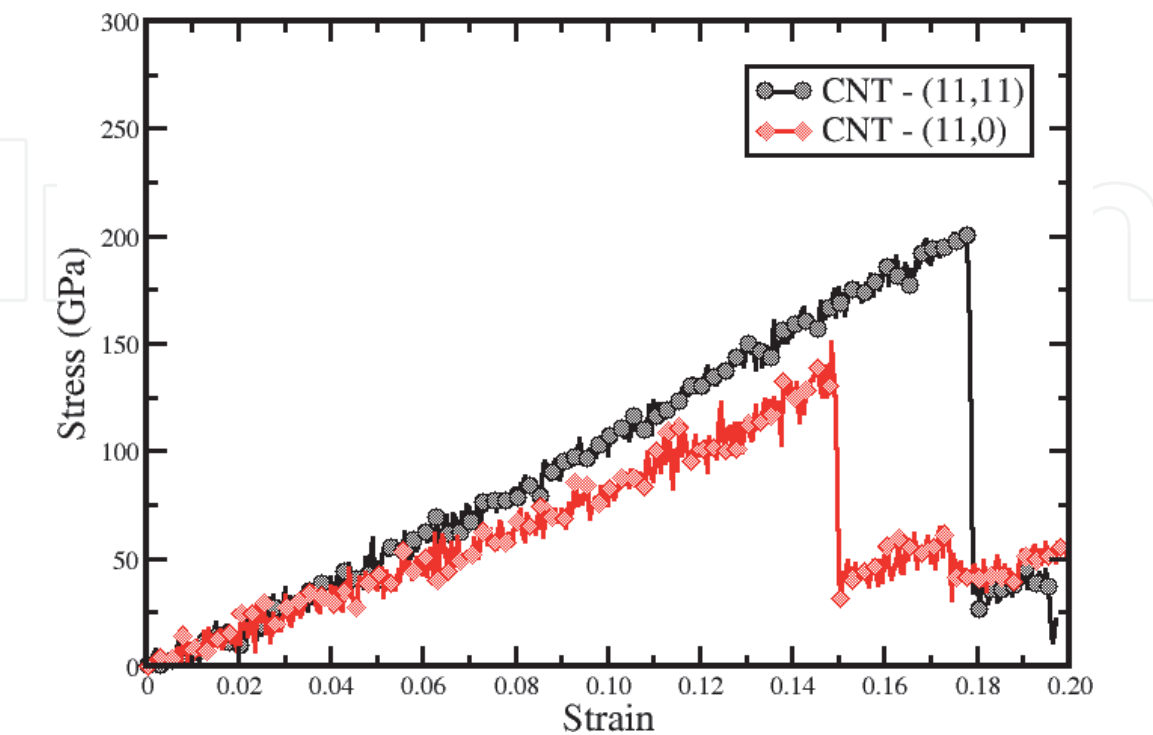
		Graphene monolayer		
	Temperature (K)	Y_{MOD} **(GPa nm)**	UTS **(GPa nm)**	**Critical strain**
X-Direction	300	3.14 ± 3.60	16.19 ± 0.03	0.10
	600	273.20 ± 3.17	15.63 ± 0.02	0.10
	1000	243.87 ± 2.27	14.76 ± 0.04	0.09
Y-Direction	300	3.13 ± 3.66	16.53 ± 0.02	0.13
	600	273.79 ± 3.37	15.86 ± 0.03	0.12
	1000	273.80 ± 2.88	15.86 ± 0.03	0.09

Table 1.
Mechanical properties values for graphene monolayer obtained by reactive molecular dynamics simulations with interatomic reactive potential ReaxFF calculated over a linear limit of 3%.

Figure 7.
Representative MD snapshots of a tensile stretch of conventional CNTs (armchair (11, 11) (top) and zigzag (11, 0) (bottom)). (a and d) Lateral view of the strained nanotube colored accordingly to the von Mises stress values (low stress in blue and high stress in red). (b and e) Zoomed view of the starting of bond breaking. (c and f) CMD-ReaxFF snapshot of the CNTs just after fracture [29].

Figure 8.
Graphical representation of stress-strain curves obtained by CMD-ReaxFF for CNTs (11, 11)—black color and CNT (11, 0)—red color, at room temperature [29].

chains along the direction of the nanotube main axis. The fracture starts from the bonds parallel and nearly parallel to the nanotube main axis for the zigzag and armchair CNTs, respectively. Because CNTs lack the acetylene chains, the structure is more rigid, the stress is accumulated directly on the hexagonal rings, the critical strains are smaller, and the ultimate strength value is larger [29]. The obtained Young's modulus (see **Figure 8**) of the (11, 11) and (11, 0) CNTs were 955 GPa and 710 GPa, respectively. The ultimate tensile strength (UTS) 166 GPa and 122 GPa and $\sigma C = 18\%$ and $\sigma C = 16\%$ in good agreement with the average value of single-walled CNTs obtained by Krishnan et al. [30].

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