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Pour l'obtention du diplôme de :

MASTER EN PHYSIQUE

Spécialité : Physique des Polymères

Par :

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Sur le thème

Study of the Deformation of an Entangled Polymer Chain using a Molecular Dynamic Program

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Soutenu en vidéoconférence le 30 juin 2021 à Tlemcen devant le jury composé de :

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Dedication

To my dearest mother « Aicha »

No dedication, dearest mother, could express the depth of feelings to you , your innumerable sacrifices and your devotion have been an encouragement to me. You have watched over my steps, and have scovered me with tenderness, your prayer and your blessing were great help to me to carry out my studies.

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Your kindness, your precious support, your encouragement throughout my years of study, your love and affection have been for me the example of perseverance.I find in you the advice of a brother and the support of a friend. may God protect you, grant you health, success and happiness in your life.

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For all the family **Derdarine** and **Moulay el boudkhili.**

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General introduction

Polymers are the basis of important industrial goods. Their rapid production growth is caused by the necessity to replace classical materials. The word “polymer” was introduced by the Swedish chemist J. J. Berzelius. Polymer science is a relatively new discipline that deals with plastics, natural and synthetic fibers, rubbers, coatings, adhesives, sealants, etc.; all of these materials nowadays have become very common. The concept of polymersis one of the great ideas of the 20th century. It emerged in the 1920s amid prolonged controversy and its acceptance is closely associated with the name of H. Staudinger who received the Nobel Prizein 1953. Many examples of synthetic polymers can be mentioned; some everyday, like polyesters or nylons, others less known, like the ones used for medical applications for organs, degradable sutures, etc[1].

In materials science, deformation refers to modifications of the shape or size of an object due to applied forces or a change in temperature. As deformation occurs, internal inter-molecular forces arise that oppose the applied force. If the applied force is not too high, these forces resist the applied force and allow the material to resumeits original state once the load is removed.

A larger applied force may cause a permanent deformation of the material, or even structural failure. Different types of deformation may result from variations in the type of material, size, and the forces applied. Types of deformation sinclude: elastic, plastic deformation and fracture. Plastics constitute an important component of the range of materialsused in modern society. Almost all aspects of daily life involve plastics or rubber. [2][3]

On the otherside, the molecular dynamics (MD) technique employs computers to carry out virtual experiments of many-body systems by solving Newton’s equations of motion. By recording and analyzing the varying coordinates, velocities and forces of the particles in the system, the dynamical processes and statistical properties can betracked and studied in detail. Such computer experiments provide the convenience of performing tests under unusual conditions or investigating non-existing materials, and the development of more accurate and realistic interaction potential functions ensures the reliability and feasibility of the simulations. Forever, MD simulations have been widely used in theoretical studies of materials science, biophysics and biochemistry. The history of MD simulations can betraced back to the middle of the 20th century when computers became available for non-military use.

Polyacrylamide is a polymer largely applied in different domains such as water treatment, pharmacy application, the mechanical properties of this material can bestudied by the moleculardynmics simulation, foreverthe deformation of a chain of polyacrylamide was investigated using a molecular dynamics program LAMMPS [4]. This work was realized in

« réseauetgel » team in the research macromolecule laboratory LRM at the University of Tlemcen.[5][6] [7]

This manuscript is divided into three chapters:

The chapter I : general concept of polymer,which contain definitions of polymers, unit of repetition.The classification and types of polymers, mechanical properties and itisended by the uses of polymers.

The chapter II : will be devoted to molecular dynamics simulation, the aim of this method. molecular interaction, force field and the steps of MD simulation.

The chapter III : results and discussion, contains the model proposition based on acrylamide monomer, a summary about the LAMMPS, the Lennard-Jones potential, the minimization of energy and the output of the polyacrylamide deformations. So this part represent the results obtained and their discussions.

At the end, we will give the essential conclusions of this work.

References

[1] Dorel Feldman, «Polymer History,» *Designed Monomers and Polymers,* vol. 11:1, pp. 1-15, 2008.

[2] Mutha N., Patel M., Premnath V, «Plastics materials flow analysis for India,» *Resources, Conservation and Recycling,* vol. 47, pp. 222-244, 2006.

[3] Anthony L. Andrady, Mike A. Neal, «Plastics consumption,» *Philos Trans R Soc Lond B Biol ,* vol. 364(1526), 2009 Jul 27.

[4] Xin Li, Applications of Molecular Dynamics in Atmospheric and Solution Chemistry, Stockholm, Sweden: Universitetsservice US-AB , 2011.

[5] S. Hamri, D. Lerari, M. Sehailia, B. Dali Youcef, T. Bouchaour, K. Bachari, *Prediction of equilibrium swelling ratio on synthesized polyacrylamide hydrogel using central composite design modeling, Int. J. Plast. Technol.,* vol. 22, Tlemcen, physics: university of abou bekr belkaid, 2018, p. 247–261.

[6] Y.H. Bendahma, S. Hamri, M. Merad, et al.,, *Conformational modeling of the system pollutant/three-dimensional poly (2-hydroxyethyl methacrylate) (PHEMA) in aqueous medium: a new approach, Polym. Bull.,* vol. 76, Tlemcen: university of abou bekr belkaid, 2019, p. 1517–1530.

[7] A. Horri, *Etude de la solvation de réseau de polyméres à base de monoméres acryliques,* Tlemcen: Département de chimie , Université de Tlemcen , 2020.

Chapter I

General concept of polymer

1. Definitions

1.1. Definition of polymer

Polymer, the root 'mer' means a unit, and poly means many. So, any of a class of natural or synthetic substances composed of very large molecules, called macromolecules, that are multiples of simpler chemical units called monomers . [1]

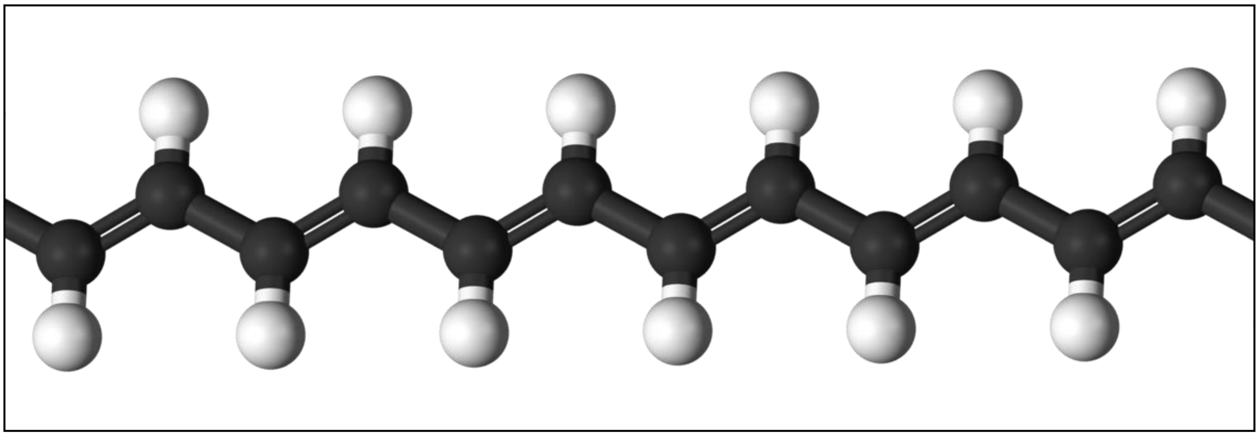

Figure 1. chain of polymer

1.2. Macromolecules

A macromolecule is a very large molecule, such as a protein. They are composed of thousands of covalently bonded atoms.

1.3. Covalent bond

A covalent bond is a chemical bond that involves the sharing of electron pairs between atoms. These electron pairs are known as shared pairs or bonding pairs, and the stable balance of attractive and repulsive forces between atoms, when they share electrons, is known as covalent bonding. [2]

1.4. Monomer

A molecule of any of a class of compounds, mostly organic, that can react with other molecules to form very large molecules, or polymers. One small macromolecule is monomers, which can react with other molecules to form very large molecules, or polymers. The essential feature of a monomer is polyfunctionality, the capacity to form chemical bonds to at least two other monomer molecules. Bifunctional monomers can form only linear, chainlike polymers, but monomers of higher functionality yield cross-linked, network polymeric products . [3]

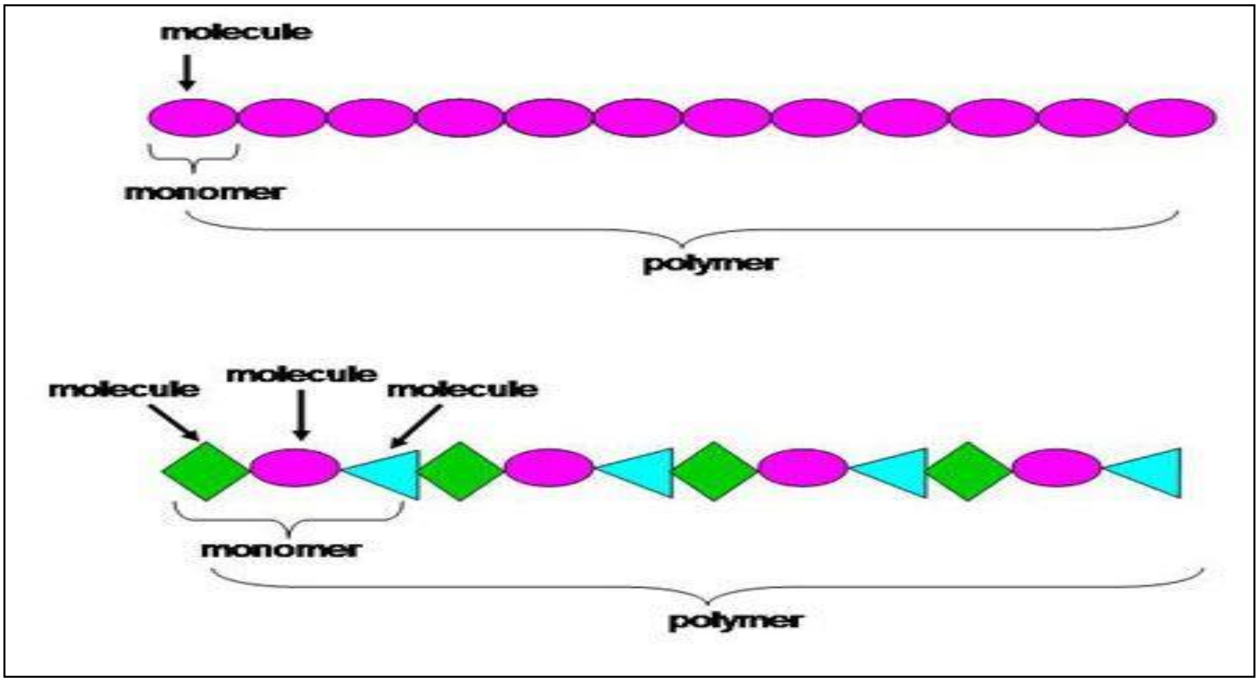

Figure 2. Polymer chain.

The word polymer designates an unspecified number of monomer units. When the number of monomers is very large, the compound is sometimes called a high polymer. Polymers are not restricted to monomers of the same chemical composition or molecular weight and structure. Some natural polymers are composed of one kind of monomer. The most natural and synthetic polymers, however, are made up of two or more different types of monomers; such polymers are known as copolymers.

Other important natural polymers include proteins, which are polymers of amino acids, and nucleic acids, which are polymers of nucleotides-complex molecules composed of nitrogen-containing bases, sugars, and phosphoric acid.

Many inorganic polymers also are found in nature, including diamond and graphite. Both are composed of carbon. In diamond, carbon atoms are linked in a three-dimensional network that gives the material its hardness. In graphite, used as a lubricant and in pencil “leads,” the carbon atoms link in planes that can slide across one another . [4]

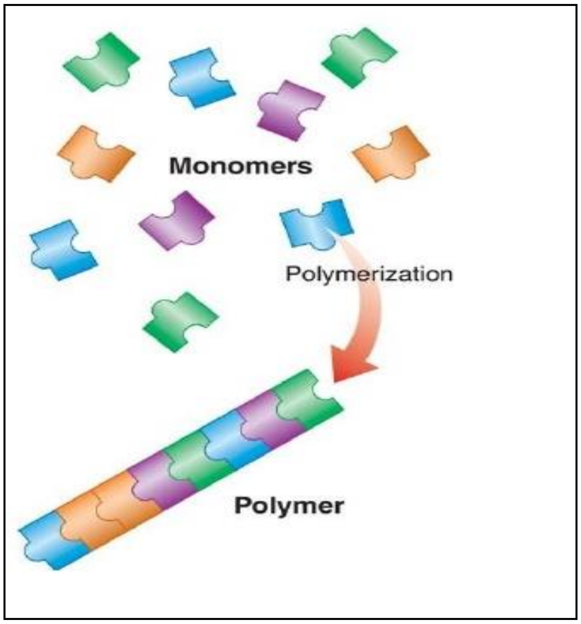

Figure 3. polymerization in polymer

1.5. Unit of polymer

An essential concept that defines polymer structure, the repeat unit or repeating unit is a part of a polymer chain whose repetition would produce the complete polymer by linking the repeat units together successively along the chain, like the beads of a necklace. [5] A repeat unit is sometimes called a mer or mer unit. "Mer" originates from the Greek word "meros," which means part. The word polymer derives its meaning from this, which means "many mers." A repeat unit, is not to be confused with the term monomer, which refers to the small molecule from which a polymer is synthesized. [6]

One of the simplest repeat units is that of the addition polymer polyvinyl chloride, -[CH_2-CHCl]n-, whose repeat unit is -[CH_2-CHCl]-. In this case, the repeat unit has the same atoms as the monomer vinyl chloride CH_2=CHCl. When the polymer is formed, the C=C double bond in the monomer is replaced by a C-C single bond in the polymer repeat unit, which links by two new bonds to adjoining repeat units. In condensation polymers, the repeat unit contains fewer atoms than the monomer or monomers from which it is formed. The subscript "n" denotes the degree of polymerization, that is, the number of units linked together.

The molecular mass of the repeat unit, MR, is simply the sum of the atomic masses of the atoms within the repeat unit. The molecular mass of the chain is just the product NMR. Other than monodisperse polymers, there is normally a molar mass distribution caused by chains of different lengths.

In copolymers, there are two or more types of repeat unit, which may be arranged in alternation, or at random, or in other more complex patterns.

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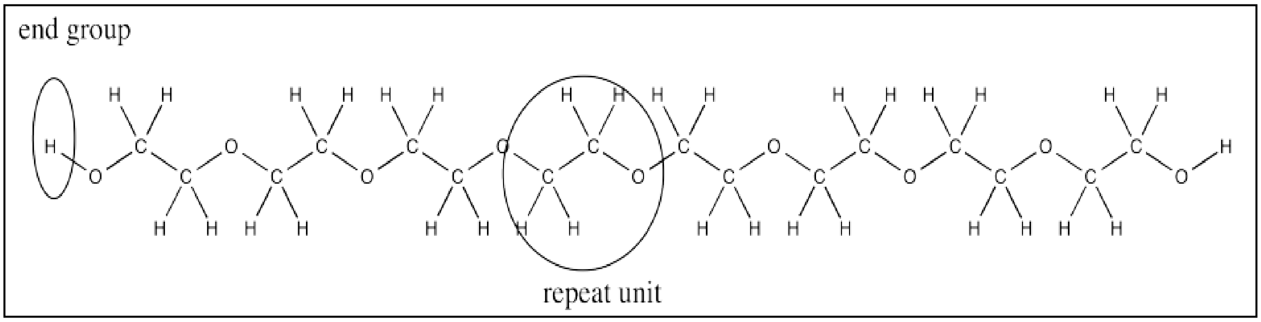


Figure 4. repeat unit in polymer

2. Types of polymers

2.1. Homopolymer

A homopolymer is a polymer where every monomer unit (mer) of the chain is the same.

2.2. Copolymer

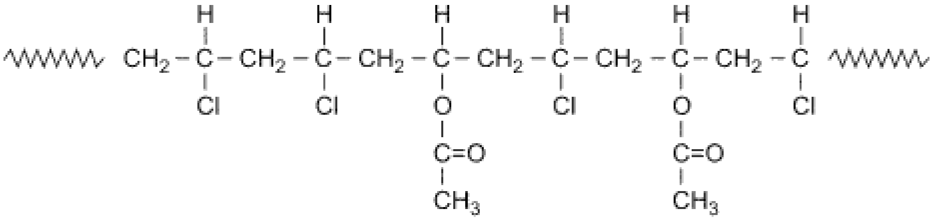
A copolymer is a polymer derived from more than one species of monomer. The polymerization of monomers into copolymers is called copolymerization. Copolymers obtained by copolymerization of two monomer species are sometimes called bipolymers. Those obtained from three and four monomers are called terpolymers and quaterpolymers, respectively .

2.3. Alternating copolymer

An alternating copolymer is a copolymer comprising two species of monomeric units distributed in an alternating sequence. The arrangement -ABABABAB- or (AB)n thus represents an alternating copolymer.

2.4. Random Copolymer

A random copolymer is one in which the monomer residues are located randomly in the polymer molecule. An example is the copolymer of vinyl chloride and vinyl acetate, made by free-radical copolymerization



1-25

Figure 5. random copolymer

2.5. Block copolymer

A block copolymer is defined as a polymer comprising molecules in which there is a linear arrangement of blocks, a block being defined as a portion of a polymer molecule in which the monomeric units have at least one constitutional or configurational feature absent from the adjacent portions.

A block copolymer is a copolymer formed when the two monomers cluster together and form 'blocks' of repeating units.

2.6. Graft copolymer

A graft copolymer is a type of copolymer in which one or more blocks of homopolymer are grafted as branches onto a main chain, meaning it is a branched copolymer with one or more side chains of a homopolymer attached to the backbone of the main chain.

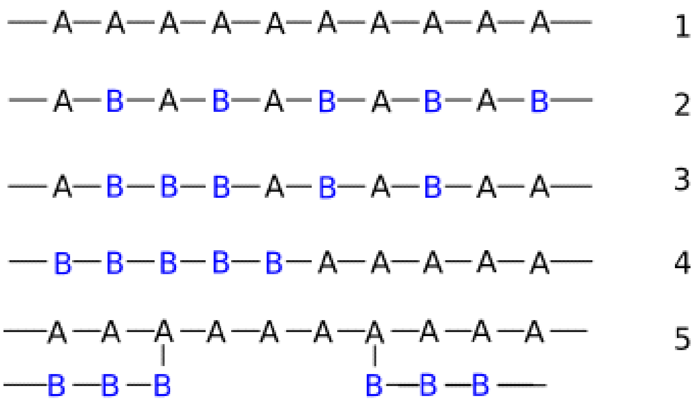


Figure 6. Different types of polymers: 1) homopolymer 2) alternating copolymer 3) random

copolymer 4) block copolymer 5) graft copolymer.

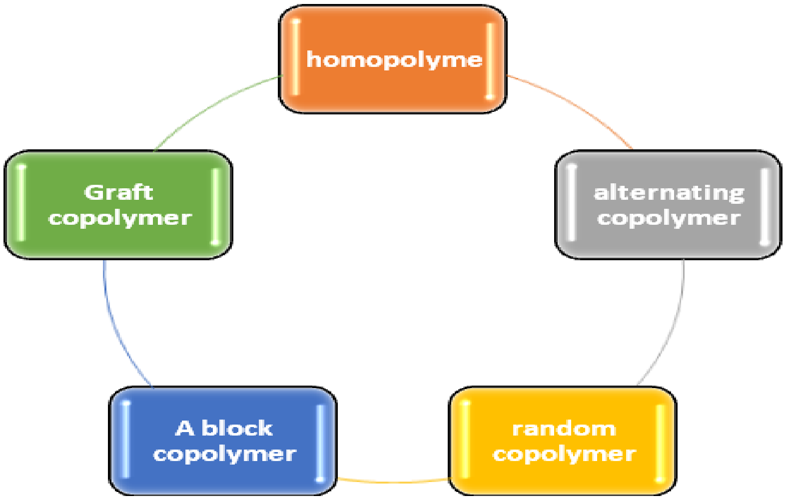


Figure 7. Different types of polymers

3. Classification of Polymers

Polymers cannot be classified under one category because of their complex structures, different behaviors and vast applications. Therefore, polymers can be classified based on the following considerations.

3.1. Classification of Polymers based on the Source of Availability

There are three types of classification under this category, namely, Natural, Synthetic, and Semi-synthetic Polymers.

3.1.1. Natural Polymers

They occur naturally and are found in plants and animals. For example proteins, starch, cellulose, and rubber. To add up, there are biodegradable polymers which are called biopolymers.

3.1.2. Semi-synthetic Polymers

Semi-Synthetic polymers are polymers obtained by making modification in natural polymers artificially in a lab. These polymers are formed by chemical reaction (in a controlled environment) and are of commercial importance. Example: Vulcanized Rubber (Sulphur is used in cross bonding the polymer chains found in natural rubber) Cellulose acetate (rayon) etc.

3.1.3. Synthetic Polymers

Synthetic polymers are polymers that humans can artificially create/synthesize in a lab. These are commercially produced by industries for human necessities. Some commonly produced polymers which we use day to day are Polyethylene (a mass-produced plastic which we use in packaging) or Nylon Fibers (commonly used in our clothes, fishing nets etc.)

3.2. Classification of Polymers based on the Structure of the Monomer Chain

This category has the following classifications:

3.2.1. Linear Polymers

These polymers are similar in structure to a long straight chain which identical links connected to each other. The monomers in these are linked together to form a long chain. These polymers have high melting points and are of higher density. A common example of this is PVC (Poly-vinyl chloride). This polymer is largely used for making electric cables and pipes.

3.2.2. Branched-chain Polymers

As the title describes, the structure of these polymers is like branches originating at random points from a single linear chain. Monomers join together to form a long straight chain with some branched chains of different lengths. As a result of these branches, the polymers are not closely packed together. They are of low density having low melting points. Low-density polyethylene (LDPE) used in plastic bags and general-purpose containers is a common example.

3.2.3. Cross-linked Polymers

In this type of polymers, monomers are linked together to form a three-dimensional network. The monomers contain strong covalent bonds as they are composed of bi-functional and tri-functional in nature. These polymers are brittle and hard. Ex: - Bakelite (used in electrical insulators), Melamine etc.

3.3. Classification Based on the types of polymerization

Any process in which relatively small molecules, called monomers, combine chemically to produce a very large chainlike or network molecule, called a polymer. The monomer molecules may be all alike, or they may represent two, three, or more different compounds. Usually at least 100 monomer molecules must be combined to make a product that has certain unique physical properties such as elasticity, high tensile strength, or the ability to form fibers that differentiate polymers from substances composed of smaller and simpler molecules; often, many thousands of monomer units are incorporated in a single molecule of a polymer. The formation of stable covalent chemical bonds between the monomers sets polymerization apart from other processes, such as crystallization, in which large numbers of molecules aggregate under the influence of weak intermolecular forces .

3-3.1. Addition Polymerization

These types of polymers are formed by the repeated addition of monomer molecules. The polymer is formed by the polymerization of monomers with double or triple bonds (unsaturated compounds). Note, in this process, there is no elimination of small molecules like water or alcohol etc (no by-product of the process). Addition polymers always have their empirical formulas the same as their monomers. Example: ethene n(CH_2=CH_2) to polyethylene -(CH_2-CH_2)n-.

3.3.2. Condensation Polymerization

These polymers are formed by the combination of monomers, with the elimination of small molecules like water, alcohol etc. The monomers in these types of condensation reactions are bi-functional or tri-functional in nature. A common example is the polymerization of Hexamethylenediamine and adipic acid. To give Nylon – 66, where molecules of water are eliminated in the process**.**

3.4. Classification Based on Monomers

3.4.1. Homopolymer

In this type, a single type of monomer unit is present. For example, Polyethene.

3.4.2. Heteropolymer or co-polymer

It consists of different types of monomer units. For example, nylon -6, 6.

3.5. Classification Based on Molecular Forces

3.5.1. Elastomers

Are rubber-like solid polymers that are elastic in nature. When we say elastic, we basically mean that the polymer can be easily stretched by applying a little force.

3.5.2. Fibres

In the classification of polymers, these are a class of polymers that are thread like in nature, and can easily be woven. They have strong inter-molecules forces between the chains giving them less elasticity and high tensile strength. The intermolecular forces may be hydrogen bonds or dipole-dipole interaction. Fibers have sharp and high melting points. A common example is that of Nylon-66, which is used in carpets and apparels.

3.5.3. Thermoplastics

Thermoplastic polymers are long-chain polymers in which inter-molecules forces (Van der Waal's forces) hold the polymer chains together. These polymers when heated are softened (thick fluid like) and hardened when they are allowed to cool down, forming a hard mass. They do not contain any cross bond and can easily be shaped by heating and using molds. A common example is Polystyrene or PVC (which is used in making pipes).

3.5.4. Thermosetting polymers

Thermosetting plastics are polymers which are semi-fluid in nature with low molecular masses. When heated, they start cross-linking between polymer chains, hence becoming hard and infusible. They form a three-dimensional structure on the application of heat. This reaction is irreversible in nature. The most common example of a thermosetting polymer is that of Bakelite, which is used in making electrical insulation. [7]

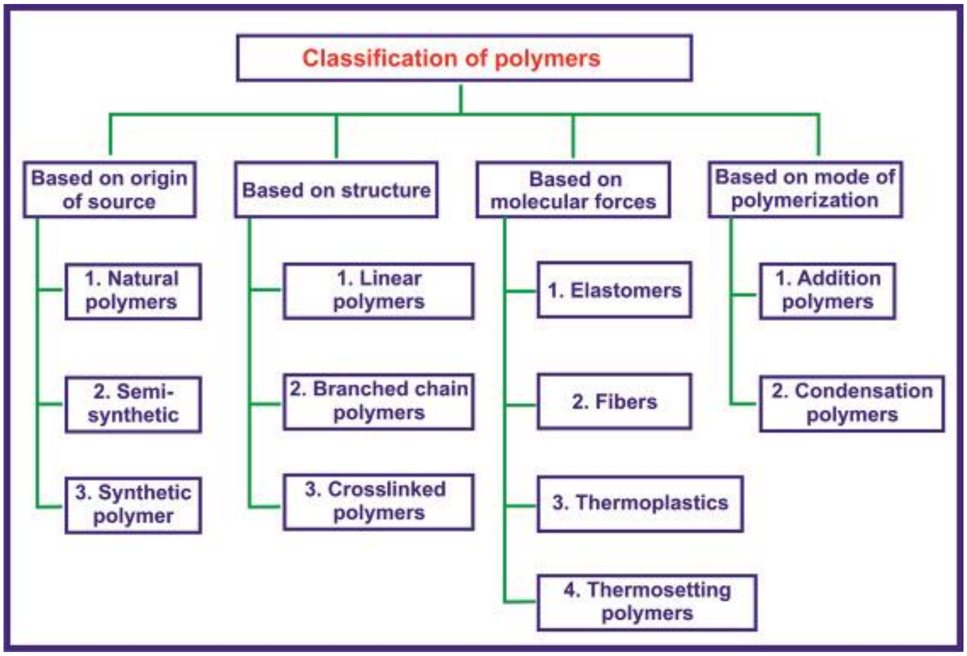


Figure 8. Classification of polymers

4. Mechanical properties

It is of great importance to be familiar with some basic mechanical properties of the material before its application in any field, such as how much it can be stretched, how much it can be bent, how hard or soft it is, how it behaves on the application of repeated load and so on.

4.1. Strength

The strength is the stress required to break the sample. There are several types of strength, namely tensile (stretching of the polymer), compressional (compressing the polymer), flexural (bending of the polymer), torsional (twisting of the polymer), impact (hammering) and so on. The polymers follow the following order of increasing strength: linear < branched < cross-linked < network.

Factors affecting the strength of polymers were as follow :

a.Molecular Weight: The tensile strength of the polymer rises with an increase in molecular weight and reaches the saturation level at some value of the molecular weight (Fig. 9). The tensile strength is related to molecular weight by the following equation**.**

$$\boldsymbol{\sigma = \sigma_\infty - \frac{A}{M} (1)}$$

$\boldsymbol{\sigma_\infty}$ is the tensile strength of the polymer with a molecular weight of infinity. A is a constant, and M is the molecular weight. At lower molecular weight, the polymer chains are loosely bonded by weak van deer Waals forces and the chains can move easily, responsible for low strength, although crystallinity is present. In the case of a large molecular weight polymer, the chains become large and hence are entangled, giving strength to the polymer.

b.Cross-linking: The cross-linking restricts the motion of the chains and increases the strength of the polymer.

c.Crystallinity: The crystallinity of the polymer increases strength, because in the crystalline phase, the intermolecular bonding is more significant. Hence, the polymer deformation can result in the higher strength leading to oriented chains.

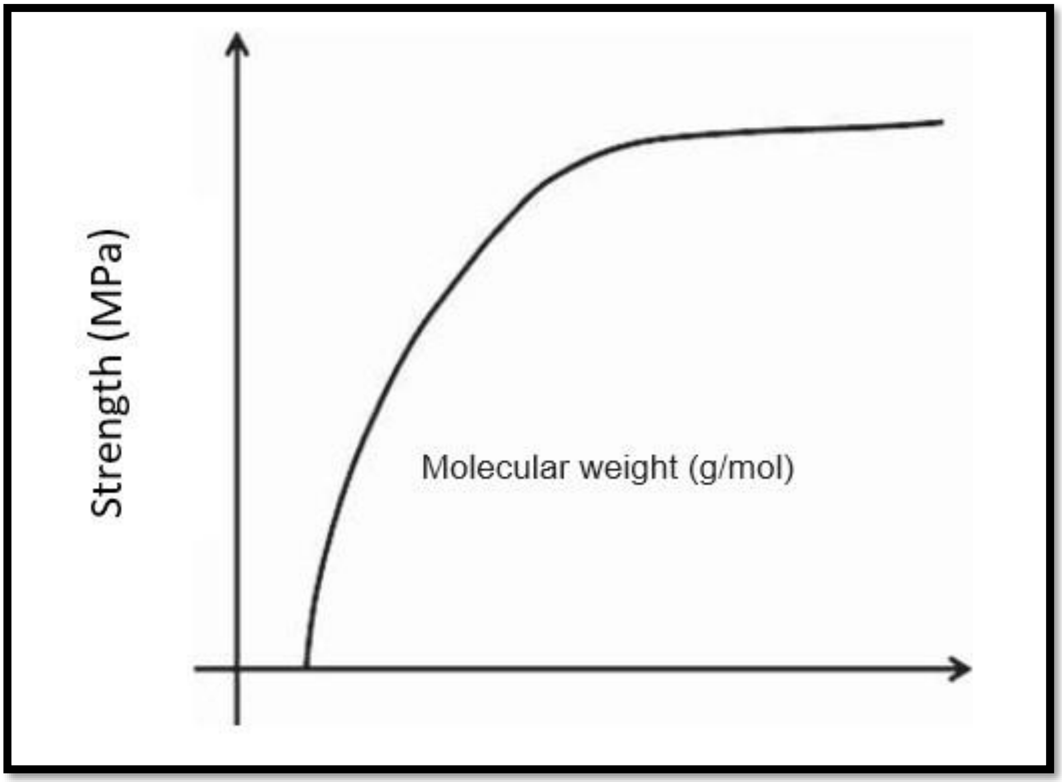


Figure 9. Variation of tensile strength with a molecular weight of the polymer**.**

4.2. Percent Elongation to Break (Ultimate Elongation)

It is the strain in the material on its breakage . It measures the percentage change in the length of the material before fracture. It is a measure of ductility. Ceramics have very low (<1%), metals have moderate (1–50%) and thermoplastic (>100%), thermosets (<5%) value of elongation to break.

4.3.Young's Modulus (Modulus of Elasticity or Tensile Modulus)

Young's Modulus is the ratio of stress to the strain in the linearly elastic region (Fig.10). Elastic modulus is a measure of the stiffness of the material.

$$\boldsymbol{E} = \frac{\boldsymbol{Tensile\ stress}\ (\boldsymbol{\sigma})}{\boldsymbol{Tensile\ strain}\ (\boldsymbol{\varepsilon})} \quad (\mathbf{2})$$

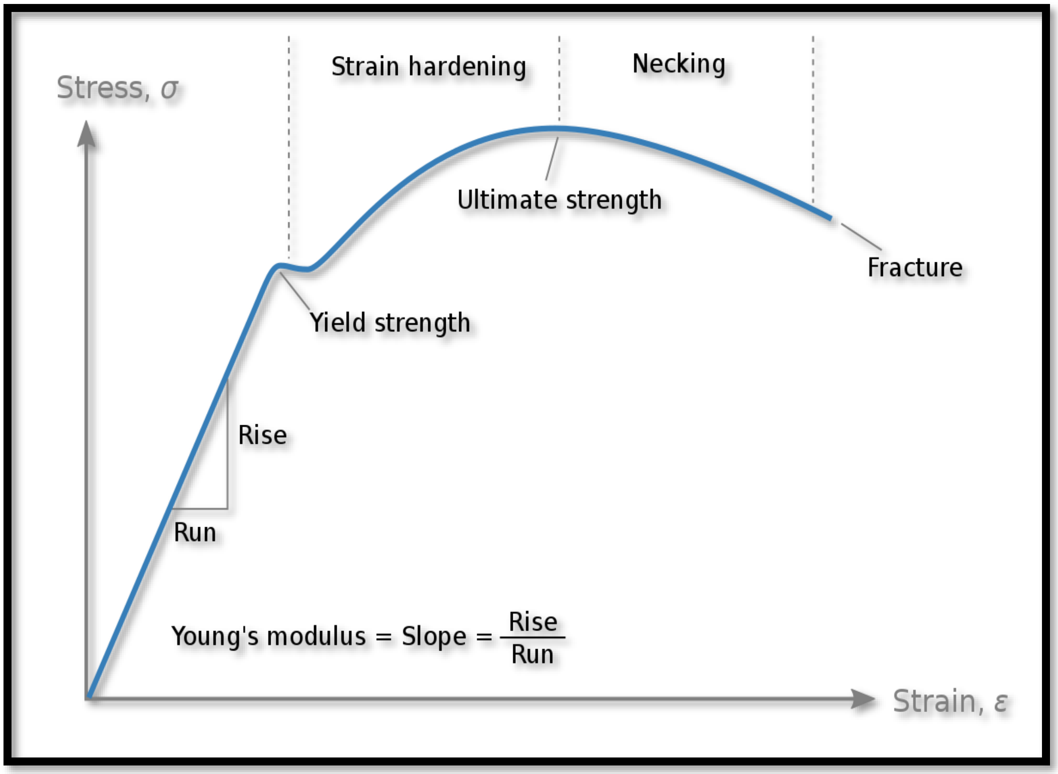


Figure 10. Young’s modulus of the polymer.

4.4.Toughness

The toughness measures the energy absorbed by the material before it breaks. A typical stress–strain curve is shown in Fig 12, which compares the stress–strain behavior of different types of materials. The rigid materials possess high Young’s modulus (such as brittle polymers), and ductile polymers also possess similar elastic modulus, but with higher fracture toughness. However, elastomers have low values of Young’s modulus and are rubbery in nature.

The toughness of a material is given by the area under a stress–strain curve (Fig11). **[8]**

$$\mathbf{Tougness} = \int \sigma \, d\varepsilon \ (3)$$

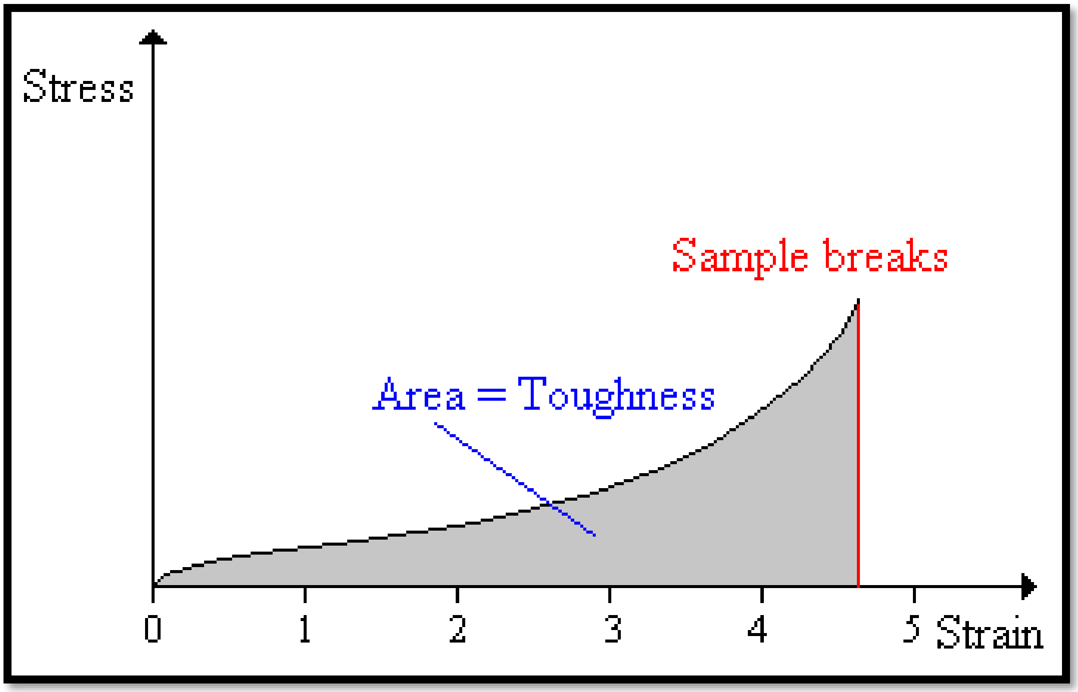
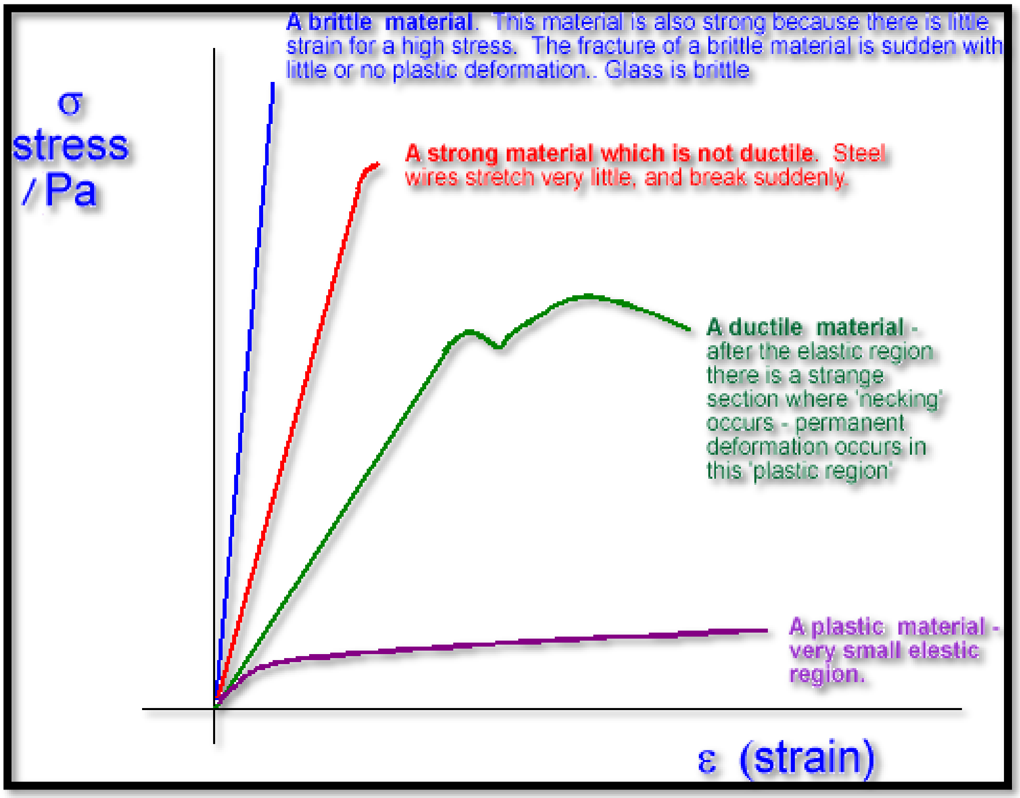


Figure 11. The toughness of polymer material



A brittle material. This material is also strong because there is little strain for a high stress. The fracture of a brittle material is sudden with little or no plastic deformation.. Glass is brittle

A strong material which is not ductile. Steel wires stretch very little, and break suddenly.

A ductile material - after the elastic region there is a strange section where 'necking' occurs - permanent deformation occurs in this 'plastic region'

A plastic material - very small elestic region.

Figure 12. Stress–strain behavior of different types of materials.

5. Uses of Polymers

The important uses of polymers in our everyday life can be summarized as follow:

- Polystyrene is one of the most common plastic, actively used in the packaging industry. Bottles, toys, containers, trays, disposable glasses and plates, tv cabinets and lids are some of the daily-used products made up of polystyrene. It is also used as an insulator.
- The most important use of polyvinyl chloride is the manufacture of sewage pipes. It is also used as an insulator in electric cables.
- Polyvinyl chloride is used in clothing and furniture and has recently become popular for the construction of doors and windows as well. It is also used in vinyl flooring.
- Urea-formaldehyde resins are used for
- making adhesives, molds, laminated sheets, unbreakable containers, etc.
- Glyptal is used for making paints, coatings, and lacquers. [9]

Figure 9. uses of polymer

References

[1] A.Augustyn , K.Rogers, «Monomer,» *The Editors of Encyclopaedia Britannica,* 2020.

[2] Campbell, N. A., Williamson, B., & Heyden, R. J., Biology: exploring life., Boston: Recording for the Blind & Dyslexic, 2006.

[3] Britannica, T., «Monomer. Encyclopedia Britannica,» 5 march 2020. [En ligne]. Available: https://www.britannica.com/science/monomer.

[4] danish kaushal, international conference on sustainable manufacturing and operations management ISOM, india, 2013, p. 134.

[5] Rudin, A., & Choi, P, The elements of polymer science and engineering, Academic press, 2012.

[6] Callister, W. D., & Rethwisch, D. G., Materials science and engineering: an introduction, New York: John Wiley & Sons, 2018.

[7] Paul C. Hiemenz,Timothy R Lodge., Polymer Chemistry Second Edition, London New York: CRC Press is an imprint of the Taylor & Francis Group, an informa business, 2007, p. 575.

[8] Kantesh Balani, Vivek Verma, Arvind Agarwal, Roger NarayanKantesh Balani, Vivek Verma, Arvind Agarwal, Roger Narayan, Biosurfaces: A Materials Science and Engineering Perspective, American ceramic society, 16 janvier 2015, p. 337.

[9] [En ligne]. Available: https://www.vedantu.com/chemistry/uses-of-polymers.

Chapter 02 :

Molecular Dynamic Simulation

1. Introduction

Molecular dynamics (MD) is a computer simulation method used in the theoretical study of biological molecules, such as proteins and nucleic acid, to analyze the physical movements of the constituent atoms and molecules. In the computer simulation, these atoms and molecules interact over time and give a sense of the dynamic evolution of the system. MD simulation mimics the changes in the structures of biological molecules over a given period, giving an atomic insights about the change in structure. This data helps to understand biological functions.

These simulations give detailed information about the fluctuations and conformational changes of the proteins and nucleic acids under study.

These methods are applied to thoroughly study the organization and dynamics of biological molecules, their complexes, and the conformational changes of proteins and nucleicacids. Many mysteries, on the femtoseconds scale, have been revealed through the study of these conformational changes.

These methods are applied in chemical physics, materials science, and biophysics. MD simulations are often used in computational biology to study protein-protein interaction, protein-ligand docking, the effects of mutation on interactions, protein folding, and flexibility of the biological molecules. Currently, it is being used to determine the tertiary structure of proteins from x-ray crystallography and NMR experiments.[1]

Figure 1. An experiment inside a computer.

2. Aim of molecular dynamics simulation

The goal of molecular dynamics simulation is to predict the behavior of atoms in a biological system and how they move as a time-dependent function thereby providing the ultimate details concerning the atoms based on algorithms of physics that govern the interatomic interactions [2] Through this, we hope to understand the properties of molecules with respect to their structure and their conduct under different conditions. It serves as an important suffix to the lab experiments thus saving time, cost, and labour of the scientists and bridges the gap between the latest technological advancements in the modern scientific community and the conventional experimental scientists. It aims at lowering the amount of guesswork and fittings traditional scientists make and helps them get an idea about the simulations that are difficult or impossible in the laboratory. We should always keep in mind that it is possible that one might not necessarily have a flawlessly realistic molecular model but the model should be able to portray the essential properties of physics and chemistry and also follow the concerned laws of mathematics along with possessing the correct biological attributes and that should be enough.

3.Concepts

Computer simulation for the study of the dynamic behavior of molecules to understand the enigma behind the complexity of the biological world is a demanding task. It necessitates the need of optimally developed models capable of mimicking the cellular environment, physical forces that can simulate the laws of physics and thermodynamics, and provide dynamicity to the model and heavy computations keeping in view the temporal aspect of the technique.

Today, tools have been developed for molecular modelling, energy calculations, algorithms to simulate the chemical aspect of the real systems, docking-scoring techniques, etc, thereby making the whole technique robust. To make the simulation realistic, the structure is placed in a "bath" of thousands of water molecules. Let us generate a fundamental idea about this incredibly amazing technology-enhanced technique.[1]

4. Molecular interaction and force field

MD simulation requires the step-by-step numerical solution of the classical equations of motion, which can in the simplest form be written as :

$$\boldsymbol{m_i r_i = f_i} \qquad \textbf{(1)}$$

where,

$$\boldsymbol{f_i = -\frac{\sigma}{\delta_{ri}} u} \qquad \textbf{(2)}$$

The forces f_i acting on the atoms derived from a potential energy U (r_N), where $r_N = (r_1, r_2, \ldots r_N)$ stands for the complete set of the geometrical 3N atomic coordinates. The force field can be understood as an empirical set of energy functions to understand the relation between energy and the interaction between atoms[3]. Typically, a Force Field is the summation of bonded and non-bonded terms or covalent and non-covalent interactions among the atoms and molecules as :

$E_{Total} = E_{Stretch} + E_{Bend} + E_{Torsion} + E_{Electrostatic} + E_{van\ der\ Waals} + E_{Hydrogen\ Bond}$ **(3)**

Each term were explained as follow :

.Bond Stretching ($E_{Stretch}$) : It describes the energy of deformation of the bond length *w.r.t.* Their equilibrium value. The energy near-equilibrium can be approximated by using Harmonic potential which does not allow the breaking of bonds [4]. The determination of the stretching force constant can be done using vibration spectroscopy.

.Angle Bending (E_{Bend}) : It describes the deformation energy of the bond angles w.r.t. their equilibrium value. The energy near-equilibrium can be approximated by using harmonic potential. This force constant can be determined by vibration spectroscopic studies.

.Torsional Term ($E_{Torsion}$) : It originates through space and accounts for the rotation of covalent bonds. This approximation of this term can be done with the help of a series of geometric functions.

.ElectrostaticTerm ($E_{Electrostatic}$) : It is calculated using Coulomb’s law with the inclusion of partial charges which are calculated by Quantum Mechanics. For better calculations, static partial charges and polarisable charges can also be taken into consideration as per one’s needs.

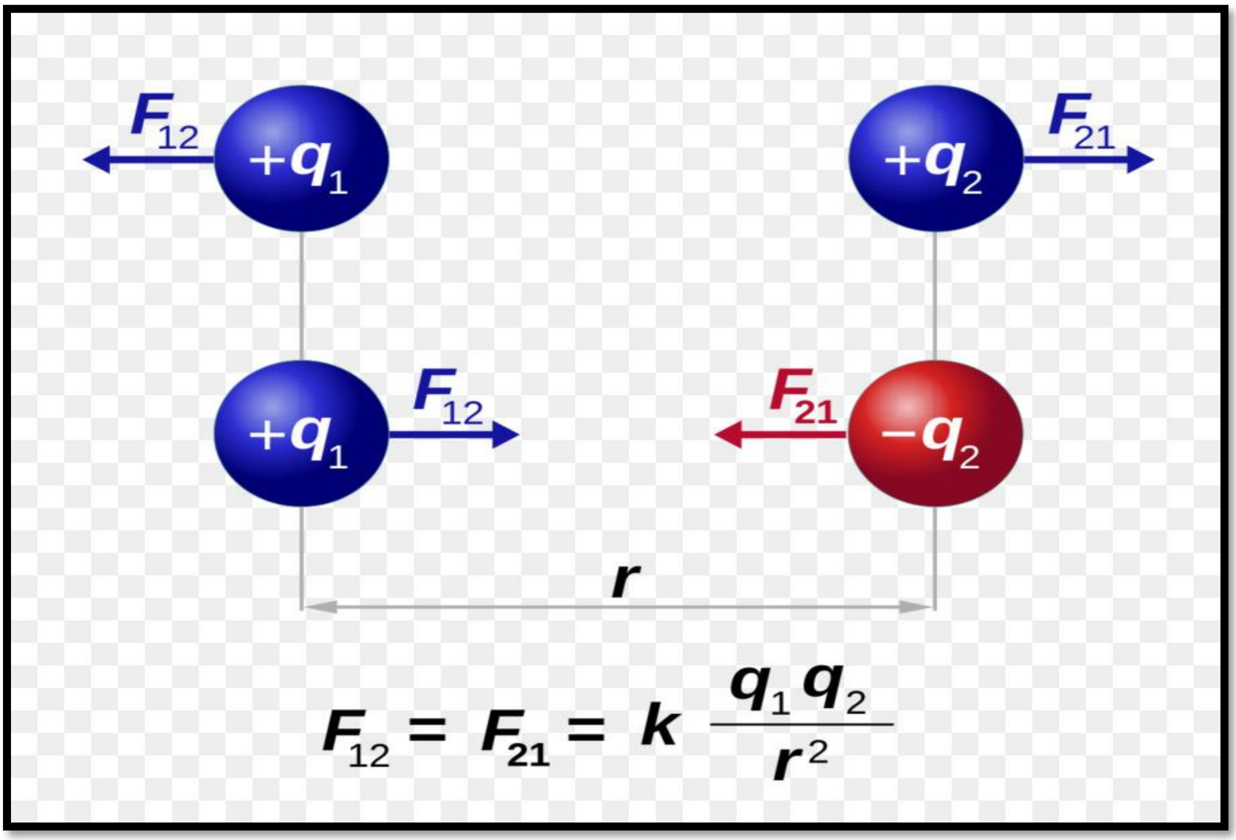


Figure 2. Coulombic interaction.

Van der Waals Term ($E_{\text{Van der Waals}}$) : It describes the interactive and repulsive interactions between atoms, in simpler terms, the interatomic forces. This term can be approximated by using Lennard Jones 12-6 potential which can be thought of as a function of the distance between the centers of the two interacting atoms/molecules.

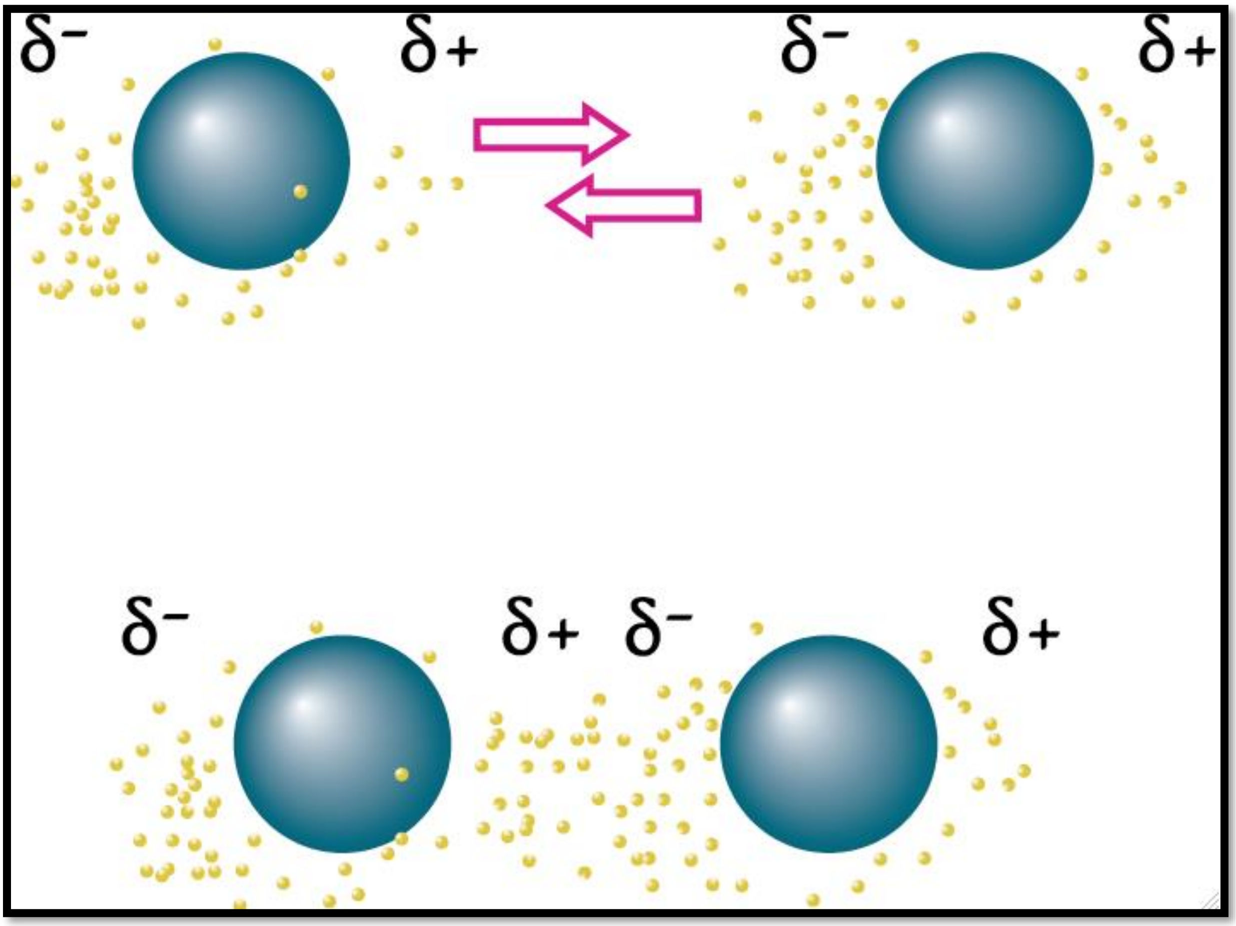


Figure 3. Van Der Waals interactions.

.Hydrogen Bond Term ($E_{\text{Hydrogen Bond}}$) : It describes the energy between atoms that have the potential to form hydrogen bonds. It is approximated by using 12-6 potential which is similar to the Lennard Jones Potential but the attractive interaction between atoms disappears faster in this case.

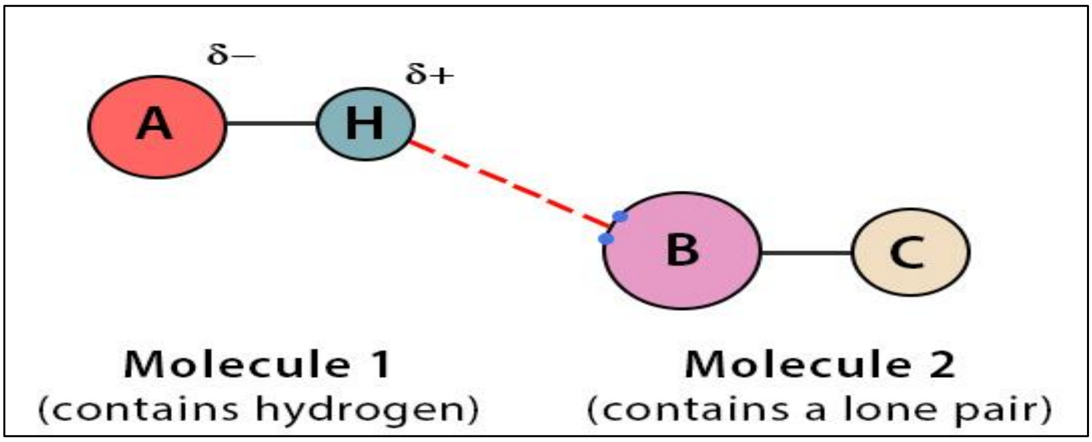


Figure 4. Hydrogen bond.

.Cross Terms : Most interaction terms studied are generally not present independently in biomolecules but affect each other. Cross term accounts for all such interactions affecting others. Cross terms include stretch-stretch, stretch-bend, bend-bend,bend-torsion, stretch torsion types of interactions.[1]

5. Periodic boundary conditions

Differential equations along with additional constraints called boundary conditions that are chosen for the approximation of a large system by using a corresponding smaller part called unit cell are known as periodic boundary conditions. Imagine the simulation of a system within a box-shaped container [5]. Since the system is physically fluid, there is a high possibility that a few particles flow out of the box due to its dynamic nature. Boundary conditions allow that whenever a particle moves out from the central box another will enter from the adjacent replica with the same speed in order to maintain a balance in the system.

To summarize, periodic boundary conditions enable a simulation to be performed using a relatively small number of particles in such a way that particles experience forces as if they are in the bulk fluid.

6. Steps of molecular dynamis simulation

6.1. Initialization:

The initial positions and the initial velocities

* Initial positions:

$$\{\boldsymbol{r_i}\}(\mathbf{0})\mathbf{i}\epsilon(\mathbf{1},\mathbf{N})$$

* Initial velocities :

$$\{\boldsymbol{v_i}\}(\mathbf{0})\mathbf{i}\epsilon(\mathbf{0},\mathbf{N})$$

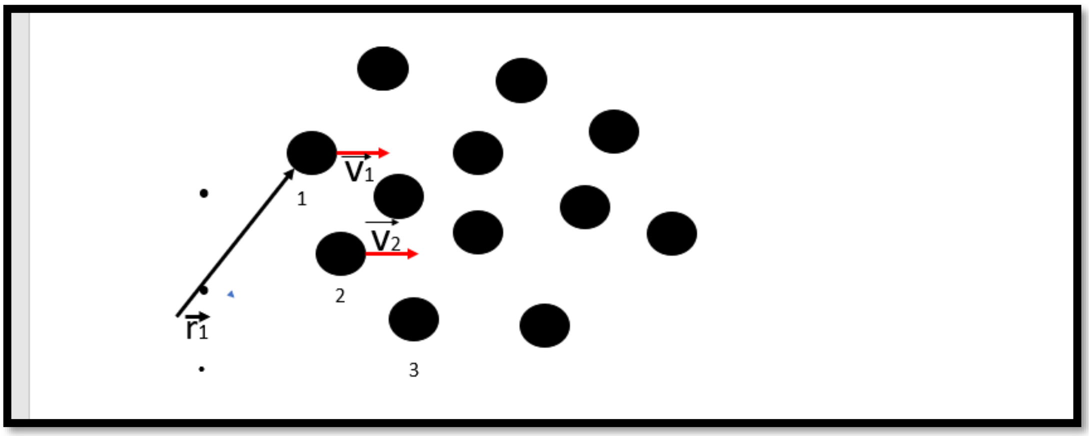


Figure 5. Initial position, Initial velocities for N atoms**.**

The initial positons of atome 1 and atome 2 permit to calculate the energy.

6.2. The energy of interactions

The energy U_{ij} of interation between atom i and atom j

$$U_{ij}(r_{ij})$$

The energy between all pairs of atoms permits to calculate the total energy of the system which will be the:

$$U_{tot} = \sum_{i>j} U_{ij} \qquad \textbf{(4)}$$

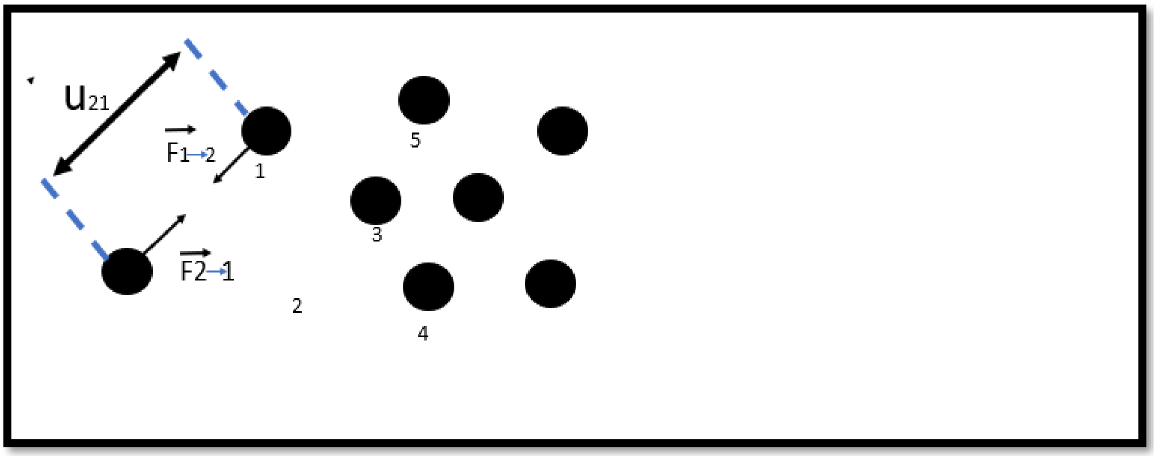


Figure 6. interatomic energy.

.Interatomic potentials : are mathematical functions to calculate the potential energy of a system of atoms with given positions in space. Interatomic potentials are widely used as the physical basis of molecular mechanics and molecular dynamics simulations in computational chemistry, computational physics and computational materials science to explain and predict materials properties.

6.3. Force calculation :

The force applied by atom j to atom i :

$$\boldsymbol{F_{ij}} = -\overrightarrow{\mathbf{grad}}\ \boldsymbol{U_{ij}} \qquad \textbf{(5)}$$

The result force applied on atom i :

$$\boldsymbol{F_i} = \sum_{j \neq \mathrm{i}} \boldsymbol{F}\mathbf{ji} \qquad \textbf{(6)}$$

6.4. Integrating the equations of motion

The Newton's law of motion is given by:

$$\boldsymbol{a_i} = \frac{\boldsymbol{f_i}}{\boldsymbol{m}} \qquad \textbf{(7)}$$

The molecular dynamics simulation method is based on Newton's second law or the equation of motion, $\boldsymbol{F} = \mathbf{ma}$, where **F** is the force exerted on the particle, **m** is its mass and **a** is its acceleration. From a knowledge of the force on each atom, it is possible to determine the acceleration of each atom in the system. Integration of the equations of motion then yields a trajectory that describes the positions, velocities and accelerations of the particles as they vary with time. From this trajectory, the average values of properties can be determined. The method is deterministic; once the positions and velocities of each atom are known, the state of the system can be predicted at any time in the future or the past. Molecular dynamics simulations can be time consuming and computationally expensive. However, computers are getting faster and cheaper.

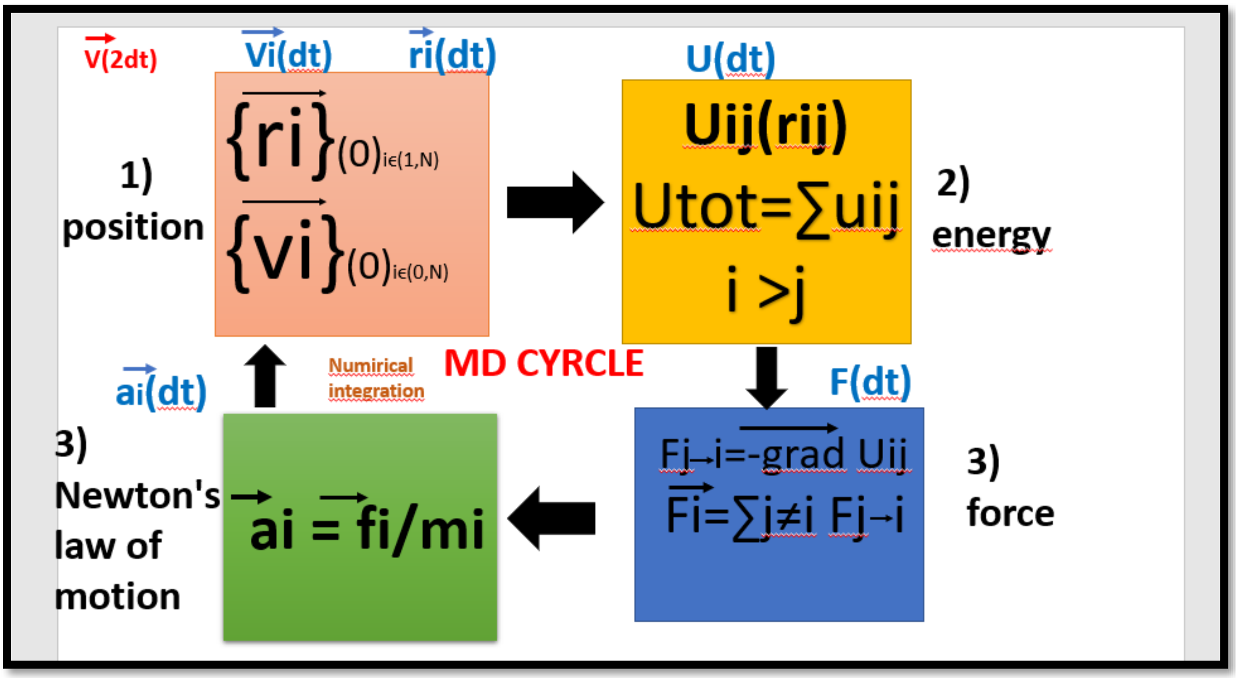


Figure 7. MD Simulation cyrcle.

Newton's equation of motion is given by :

$$\boldsymbol{F_i = m_i a_i} \qquad \textbf{(8)}$$

where F_i is the force exerted on particle i, m_i is the mass of particle i and a_i is the acceleration of particle i. The force can also be expressed as the gradient of the potential energy,

$$\boldsymbol{F_i = -\nabla_i v} \qquad \textbf{(9)}$$

Combining these two equations yields :

$$\boldsymbol{-\frac{dv}{dr_i} = m_i \frac{d^2 r_i}{dt^2}} \qquad \textbf{(10)}$$

where V is the potential energy of the system. **Newton's** equation of motion can then relate the derivative of the potential energy to the changes in position as a function of time

Newton's second law of motion: a simple application

$$\boldsymbol{F = \mathrm{m.a} = \mathrm{m}.\frac{dv}{dt} = \mathrm{m}.\frac{d^2x}{dt^2}} \qquad \textbf{(11)}$$

Taking the simple case where the accelerationis constant,

$$\boldsymbol{a} = \frac{d\boldsymbol{v}}{d\boldsymbol{t}} \quad \textbf{(12)}$$

The expression of the velocity after integration is given by :

$$\boldsymbol{v} = \mathbf{at} + \boldsymbol{v_0} \quad \textbf{(13)}$$

And since

$$\boldsymbol{v} = \frac{d\boldsymbol{x}}{d\boldsymbol{t}} \quad \textbf{(14)}$$

Integration permits to obtain the following equation :

$$\boldsymbol{x} = \mathbf{v.t} + \boldsymbol{x_0} \quad \textbf{(15)}$$

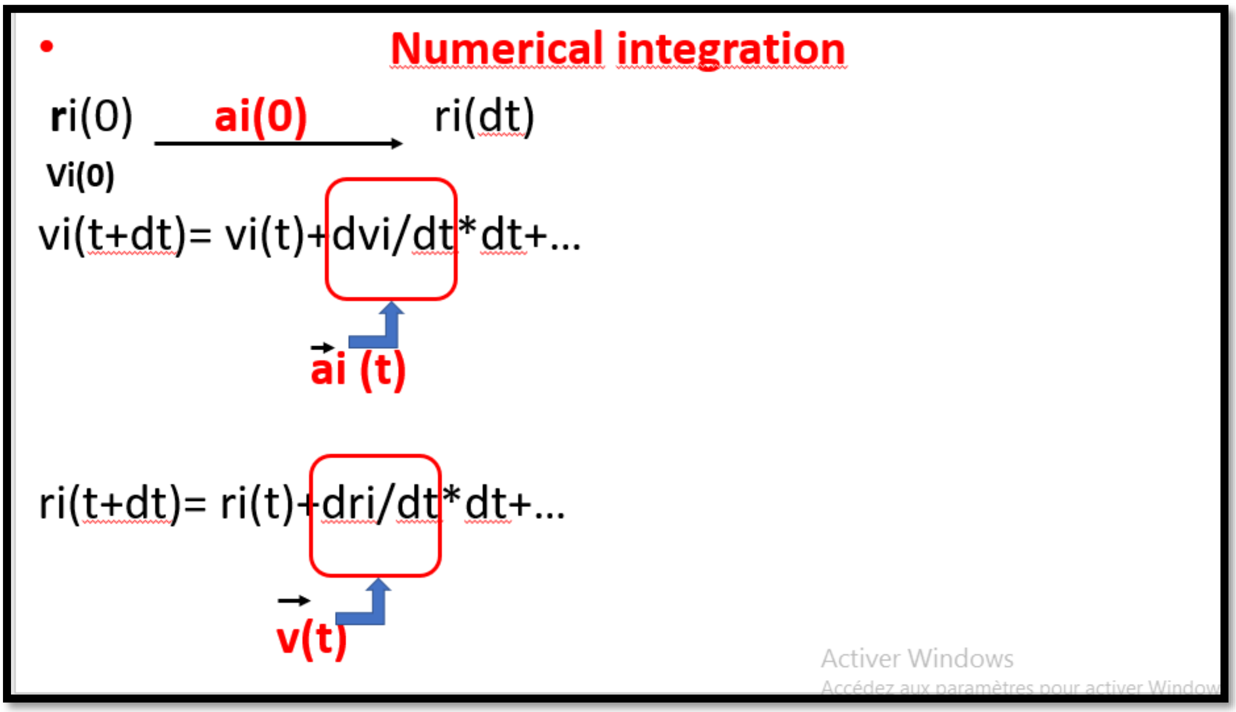
Combining this equation with the expression for the velocity, the following relation which gives the value of *x* at time *t* as a function of the acceleration, *a*, the initial position, x_0 , and the initial velocity, v_0, is given by :

$$\boldsymbol{x} = \frac{\mathbf{1}}{\mathbf{2}} * \boldsymbol{a} * \boldsymbol{t^2} + \boldsymbol{v_0} * \boldsymbol{t} + \boldsymbol{x_0} \qquad \textbf{(16)}$$

The acceleration is given as the derivative of the potential energy with respect to the position, *r*,

$$\boldsymbol{a} = -\frac{\mathbf{1}}{\boldsymbol{m}}\frac{d\boldsymbol{E}}{d\boldsymbol{r}} \qquad \textbf{(17)}$$

Therefore, to calculate a trajectory, one only needs the initial positions of the atoms, an initial distribution of velocities and the acceleration, which is determined by the gradient of the potential energy function. The equations of motion are deterministic, e.g., the positions and the velocities at time zero determine the positions and velocities at all other times, t. The initial positions can be obtained from experimental structures, such as the x-ray crystal structure of the protein or the solution structure determined by NMR spectroscopy.



- Numerical integration

ri(0) $\xrightarrow{ai(0)}$ ri(dt)

Vi(0)

vi(t+dt)= vi(t)+$\boxed{dvi/dt}$*dt+…

$\vec{ai}$ (t)

ri(t+dt)= ri(t)+$\boxed{dri/dt}$*dt+…

$\vec{v}$(t)

Figure 8. Numericalintegration.

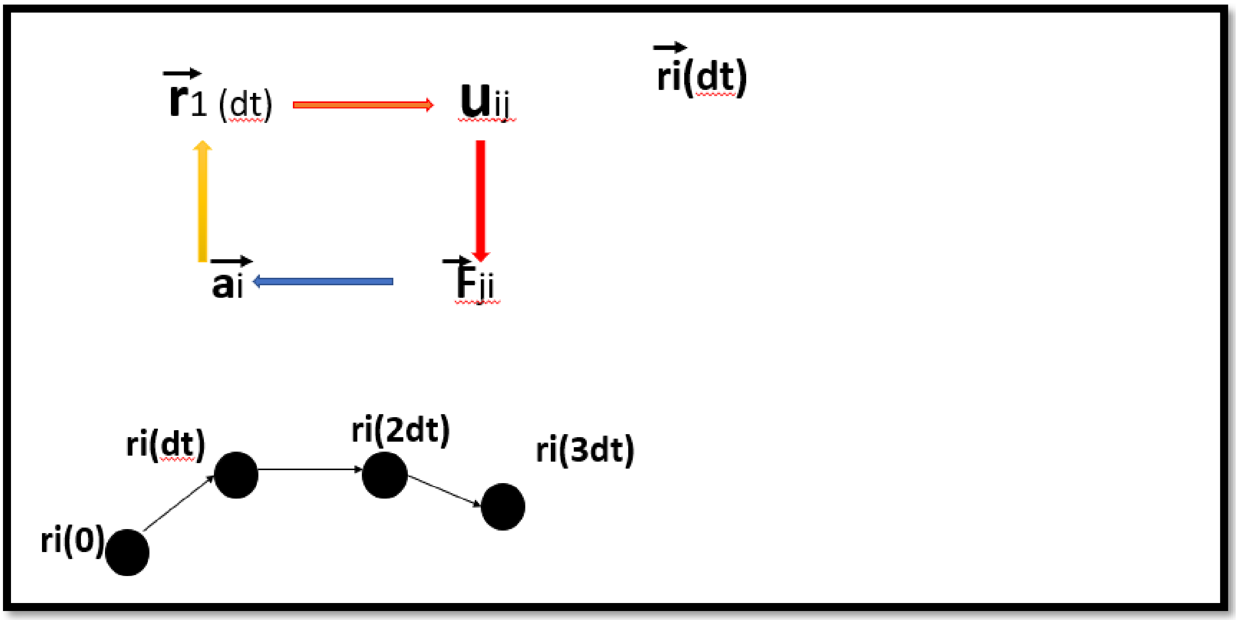


Figure 9. Cycle of MD simulation.

7. **Conclusions**

LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, or macroscopic systems using a variety of interatomic potentials (force fields) and boundary conditions. It can model 2d or 3d systems with only a few particles up to millions or billions. [6]

References

[1] Mohammad Sufian Badar, et al, Molecular Dynamics Simulations: Concept, Methods, and Applications, 12 August 2020.

[2] Hollingsworth, s. A., and dror, r. O., «Molecular dynamics simulation for all.,» *Neuron,* vol. 99 (6), pp. 1129-1143, 2018.

[3] Mayo, S. L., Olafson, B. D., and Goddard, W. A., «DREIDING: a generic force field for molecular simulations.,» *Journal of Physical chemistry ,* vol. 94 (26), pp. 8897-8909, 1990.

[4] Pearlman, D. A., and Kollman, P. A., «The overlooked bond-stretching contribution in free energy perturbation calculations.,» *The Journal of chemical physics,* vol. 94 (6), pp. 4532-4545, 1991.

[5] Karaa,W.B.A , Biomedical Image Analysis and Mining Techniques for Improved Health Outcomes, IGI Global, November 3, 2015.

[6] « Overview of LAMMPS,» 2003-2020. [En ligne]. Available: https://docs.lammps.org/Intro_overview.html.

Chapter 3 :

Results and Discusson

1.introduction

The changes in materials dimensions in response to mechanical forces is called deformation, we have done a study about the deformation of polyacrylamide chain, firstly, software used in this study are presented, the lennard jones potential is explained, because the model " polyaccrylamide" contain atomes and lj potential helps us to understand the interaction between them. The description of Lammps program has done also because it allowed us to write the script of deformation and minimization, the output results were represented on curves and were all explained.

2-software

a-.Avogadro

Avogadro is an advanced molecular editor designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science and related areas. It offers a flexible rendering framework and a powerful plugin architecture. [1]

b-.Lammps

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a molecular dynamics program from Sandia National Laboratories. LAMMPS makes use of Message Passing Interface (MPI) for parallel communication and is free and open-source software, distributed under the terms of the GNU General Public License.

LAMMPS is a classical molecular dynamics (MD) code that models ensembles of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, solid-state (metals, ceramics, oxides), granular, coarse-grained, or macroscopic systems using a variety of interatomic potentials (force fields) and boundary conditions. It can model 2d or 3d systems with only a few particles up to millions or billions.

LAMMPS can be built and run on a laptop or desktop machine, but is designed for parallel computers. It will run on any parallel machine that supports the MPI message-passing library. This includes shared-memory boxes and distributed-memory clusters and supercomputers. [2]

3-Monomer and model

a-**Acrylamide:** 2-propenamide, ethylenecarboxamide, acrylicacid amide, vinylamide, propenoicacid amide. Acrylamide appears as a white crystalline solid, Acrylamide is a reactive chemical, which is used as monomer in the synthesis of polyacrylamides used e.g. in purification of water . Acrylamide occurs through radical reactions with the double bond. [3]

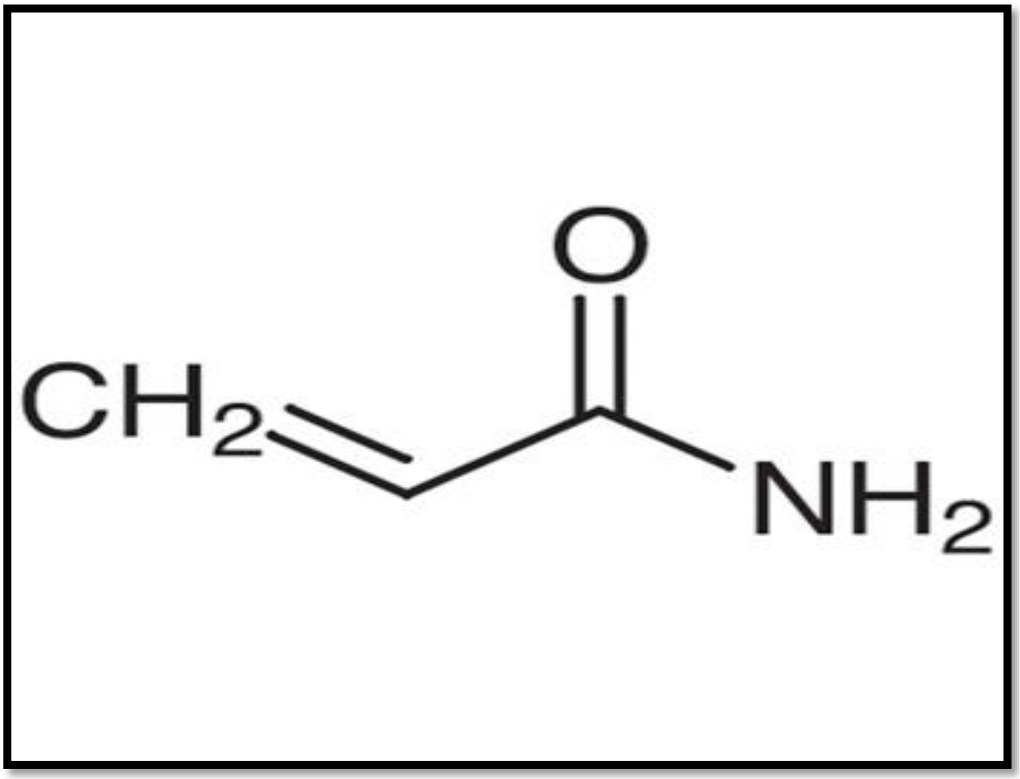
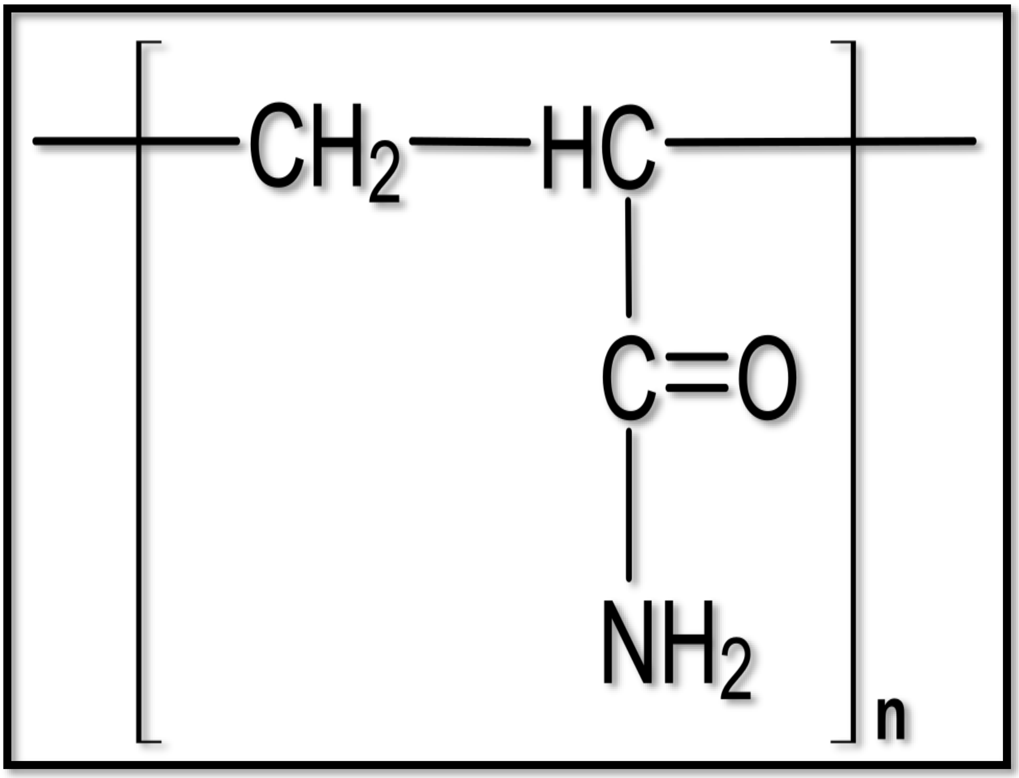


Figure 1. Acrylamide structure.

b-Polyacrylamide :

Polyacrylamide is a polymer with the formula [-CH_2-CH(-$CONH_2$)-]n, formed from acrylamide. It can be cross-linked by incorporating into the polymerization mixture a bifunctional derivative of acrylamide: N,N'-methylene-bis-acrylamide (CH_2=CH-CO-NH-$)_2CH_2$.



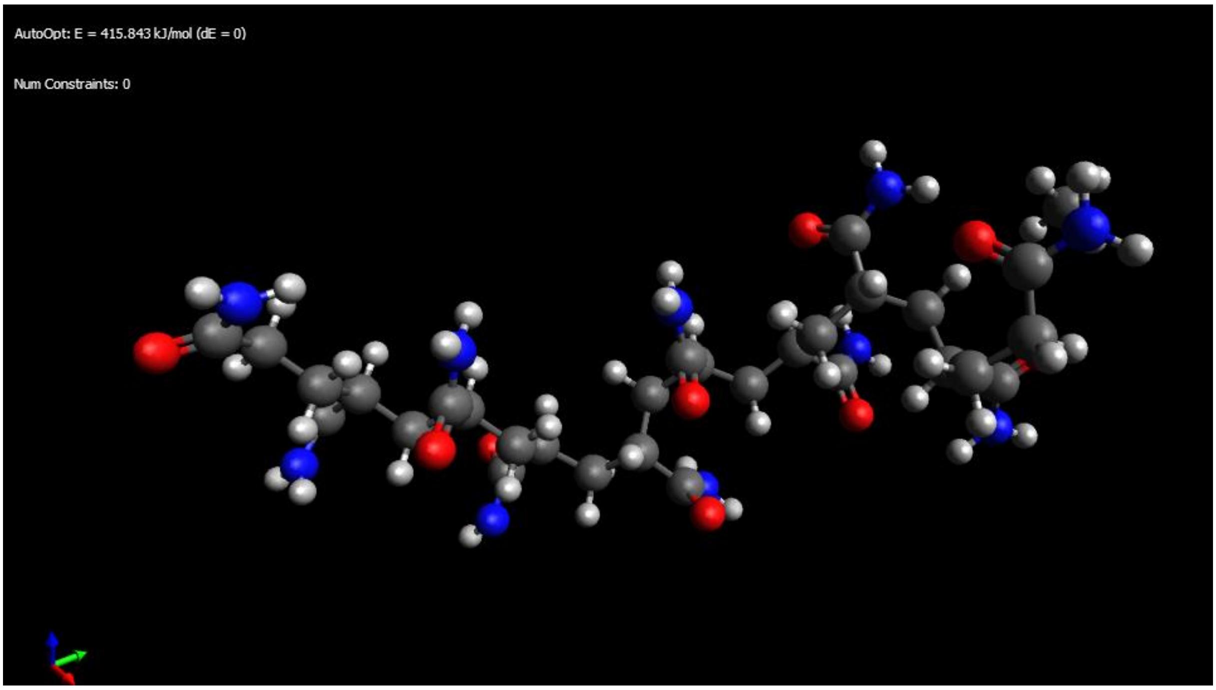
$$\left[\,-CH_2-\underset{\underset{\displaystyle NH_2}{|}}{\underset{\displaystyle C=O}{|}}{HC}-\,\right]_n$$

Figure 2. Polyacrylamide structure.

c-Model proposition

A polyacrylamide model with 10 monomers of acrylamide using avogadro is prepared.

After that we have optimize geometry of polyacrylamide chain, the avogadro permits to calculate the minimum of energy which is like we see in the figure E = 415.843 KJ/mol (dE = 0)



```
AutoOpt: E = 415.843 kJ/mol (dE = 0)

Num Constraints: 0
```

Figure 3. Energy minimization of the polyacrylamide.

4- The Lennard-Jones potential

The Lennard-Jones potential describes the potential energy of interaction between two non-bonding atoms or molecules based on their distance of separation. The potential equation accounts for the difference between attractive forces (dipole-dipole, dipole-induced dipole, and London interactions) and repulsive forces.

Imagine two rubber balls separated by a large distance. Both objects are far enough apart that they are not interacting. The two balls can be brought closer together with minimal energy, allowing interaction. The balls can continuously be brought closer together until they are touching. At this point, it be comes difficult to further decrease the distance between the two balls. In order to bring the balls any closer together, increasing amounts of energy must beadded. This is because eventually, as the balls begin to invade each other’s space, they repel each other; the force of repulsionis far greater than the force of attraction. This is similar to that which takes place in neutral atoms and molecules and is often described by the **Lennard-Jones potential**.

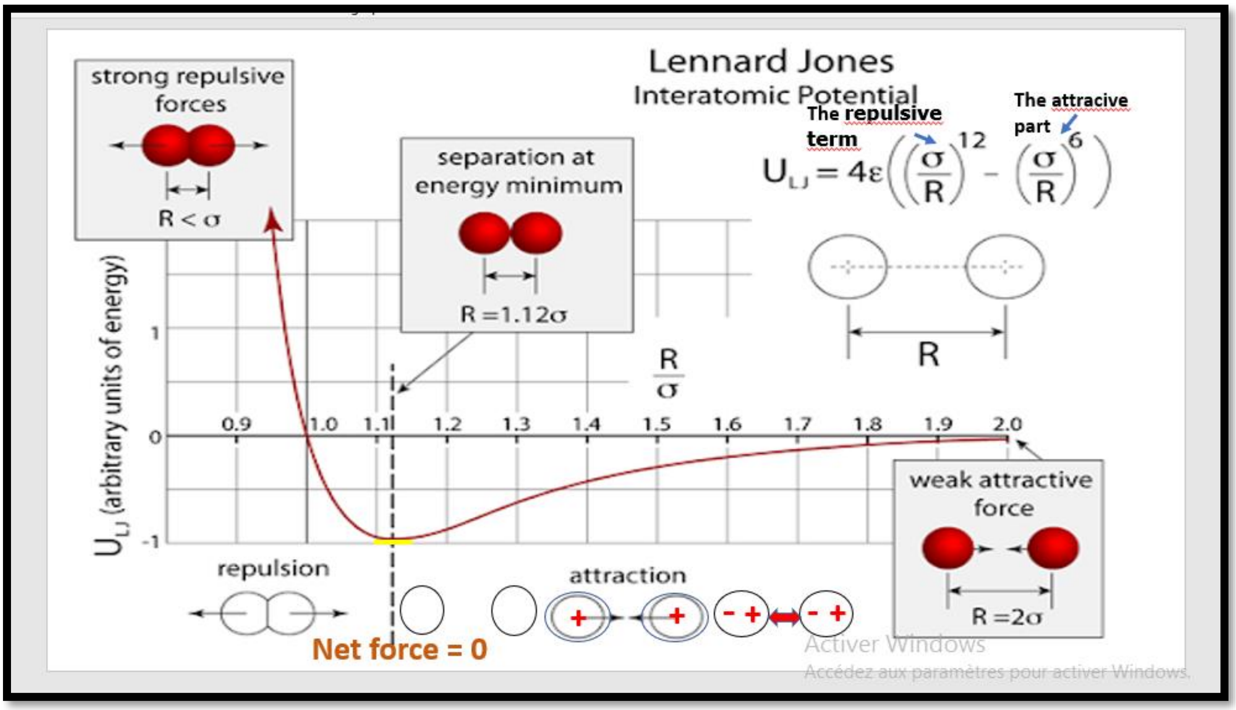


Figure 4. Interaction in The Lennard-Jones curve.

The Lennard-Jones model consists of two 'parts';as teep repulsive term, and smo other attractive term, representing the London dispersion forces. Apart from being an important model in itself, the Lennard-Jones potential frequently forms one of 'building blocks' of many force fields. It is worth mentioning that the 12-6 Lennard-Jones model is not the most faithful representation of the potential energy surface, but rather its use is widespread due to its computational expediency.The Lennard-Jones Potential is given by the following equation : $\mathbf{V(r) = 4\epsilon[(\sigma r)12 - (\sigma r)6](1)(1)V(r) = 4\epsilon[(\sigma r)12 - (\sigma r)6]}$ $\mathbf{(1)}$

Or is sometimes expressed as

$\mathbf{V(r) = Ar12 - Br6(2)(2)V(r) = Ar12 - Br6}$ $\mathbf{(2)}$

Where :

- VV is the intermolecular potential between the two atoms or molecules.
- ϵϵ is the well depth and a measure of how strongly the two particles attract each other.
- σσ is the distance at which the intermolecular potential between the two particles is zero σσ gives a measurement of how close two nonbonding particles can get and is thus referred to as the *van der Waals radius*. It is equal to one-half of the internuclear distance between nonbonding particles.
- rr is the distance of separation between both particles (measured from the center of one particle to the center of the other particle).
  [4] [5]

5-Energy minimization

Energy minimization (also called energy optimization, geometry minimization, or geometry optimization) is the process of finding an arrangement in space of a collection of atoms where, according to some computational model of chemical bonding, the net inter-atomic force on each atom is acceptably close to zero and the position on the potential energy surface (PES) is a stationary point.

Using LAMMPS program, command integrated in lammps permits to minimize the polyacrylamide chain, the output results were represented on the figure below. The cut of is varied to see the behavior of energy in response to the time.

a- Case with Cut=10.5 :

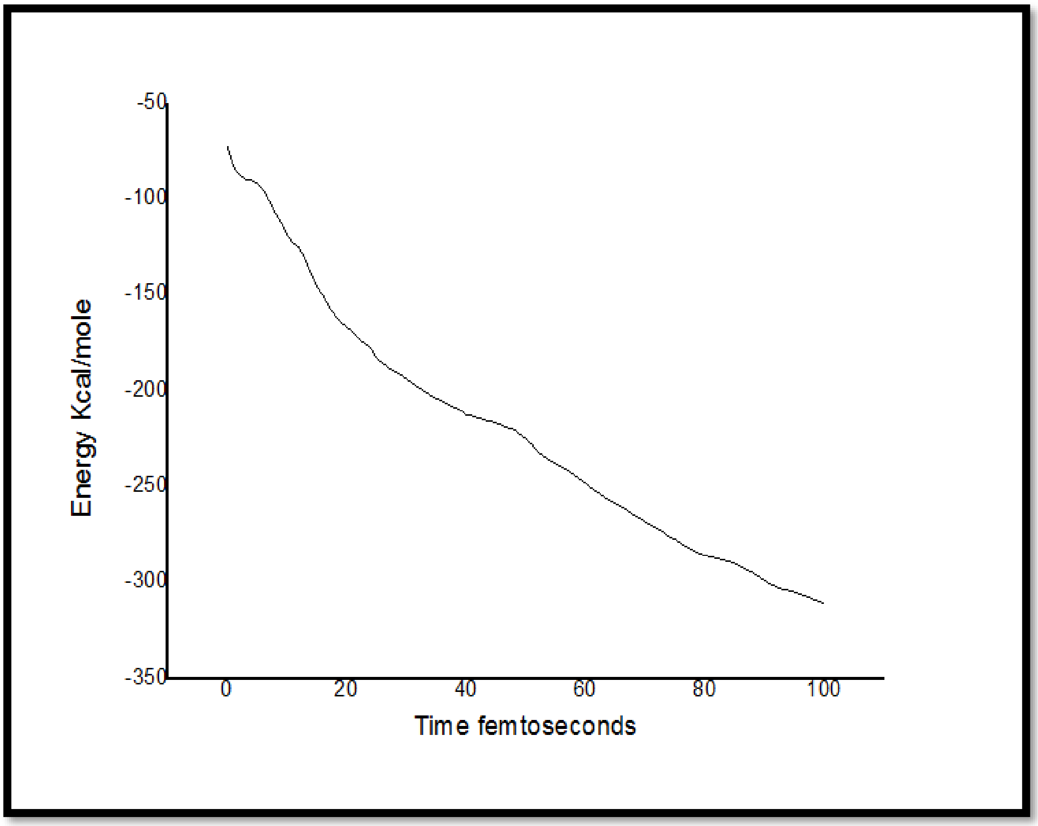


Figure 5. Energy as a function of time « cut=10.5 ».

b- Case with Cut=12 :

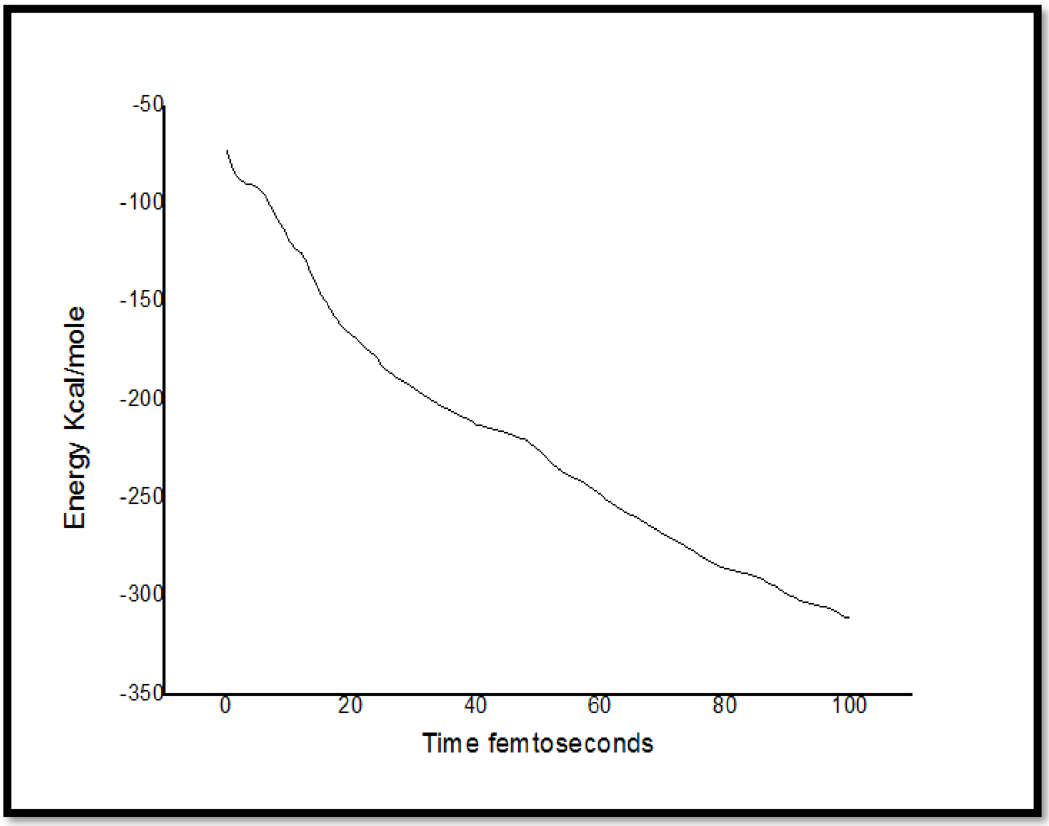


Figure 6. Energy as a function of time « cut=12 ».

The graphes represented on figures 5 and 6 shows the variation of energy as a function of time.

In this curves we notice that the energy decreases with time ,we also notice that the curves are almost the same although we changed the cut once 10.5 an other time 12.

6-Deformation

As deformation occurs, internal inter-molecular forces arise that oppose the applied force. If the applied force is not too high, these forces resist the applied force and allow the material to resume its original state once the load is removed. A larger applied force may cause a permanent deformation of the material, or even structural failure.

Types of deformation are given as follow :

a- Plastic deformation

a material changes shape when a stress is applied to it and does not go back to its original state when the stress is removed.

b- Elastic deformation

In elastic deformation a material changes shape when a stress is applied to it but goes back to its original state when the stress is removed.

Unlike the case of elastic deformation, these changes of shape in the material are irreversible. An object in the plastic deformation range will first have undergone elastic deformation, which is reversible, so the object will return part way to its original shape.

In elastic deformation a material changes shape when a stress is applied to it but goes back to its original state when the stress is removed. [6]

c- Fracture

occurs when a structural component separates into two or more pieces.

6.1. Stress-strain curve of polyacrylamide

a-Stress : In mechanics, stress is defined as a force applied per unit area. It is given by the formula :

$$\boldsymbol{\sigma = \frac{F}{A}} \qquad (\mathbf{3})$$

where,

σ is the stress applied
F is the force applied
A is the area of force application
The unit of stress is N/m2

Stress applied to the polyacrylamide model is the tensile stress**,** It is the force applied per unit area which results in the increase in length (or area) of a body. Objects under tensile stress become thinner and longer as you can see on the figure below. The tensor of pressure included in LAMMPS permits to define the stress in our case.

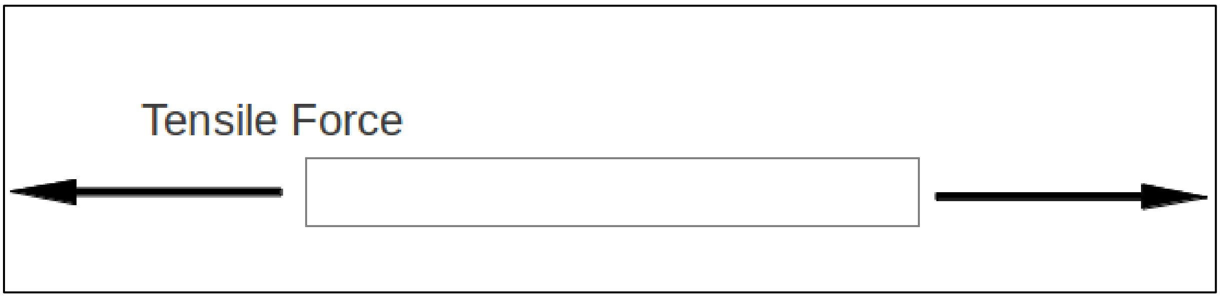


Figure 7. The tensile stress.

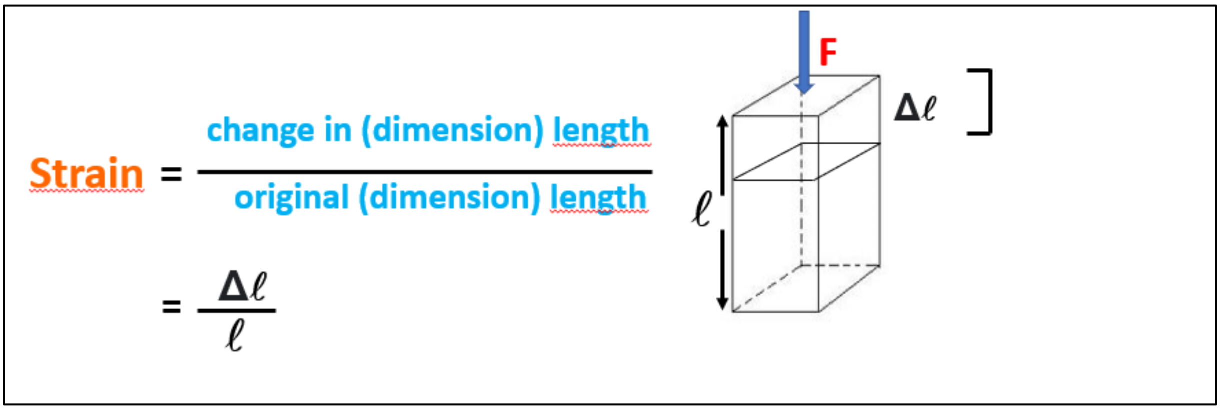
b- Strain

According to the strain definition, it is defined as the amount of deformation experienced by the body in the direction of force applied, divided by initial dimensions of the body. The relation for deformation in terms of length of a solid is given below.

$$\boldsymbol{\epsilon = \frac{\delta l}{L}} \qquad (\mathbf{4})$$

where,
ϵ is the strain due to stress applied
δl is the change in length
L is the original length of the material.

The strain is a dimension less quantity as it just defines the relative change in shape. Depending on stress application, tensile strain is the change in length (or area) of polyacrylamide chain due to the application of tensile stress. Using Lammps program, the tensile strain is included in the script to calculate the deformation percentage.



$$\text{Strain} = \frac{\text{change in (dimension) length}}{\text{original (dimension) length}}$$

$$= \frac{\Delta\ell}{\ell}$$

Figure 8. Strain definition.

The relation between stress and strain is that they are directly proportional to each other up to an elastic limit. Hooke’s law explains the relationship between stress and strain. According to Hooke’s law, the strain in a solid is proportional to the applied stress and this should be within the elastic limit of that solid.

The include of all information, the potential type, the strain expression, in the Lammps script permit to get the strain versus stress curve, for two cases, as you can see below.

a- Case with Cut=10.5 :

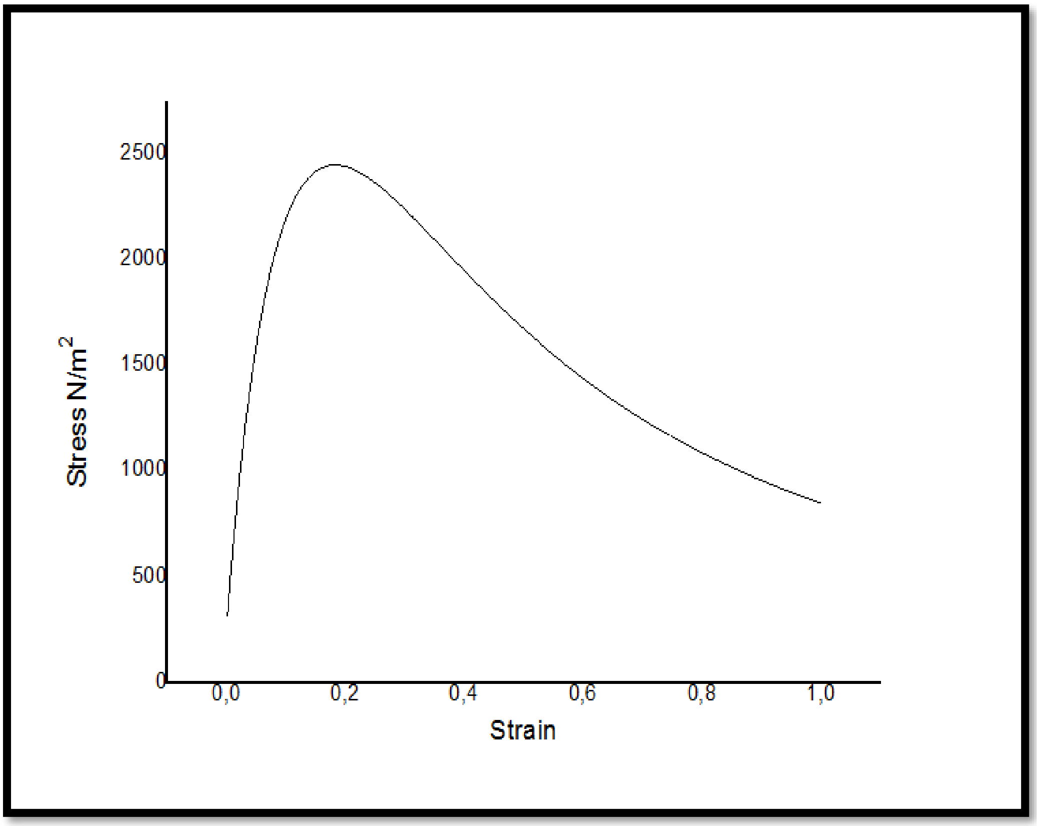


Figure 9. Stress Strain curve of a polyacrylamide.

b- Case with Cut=12 :

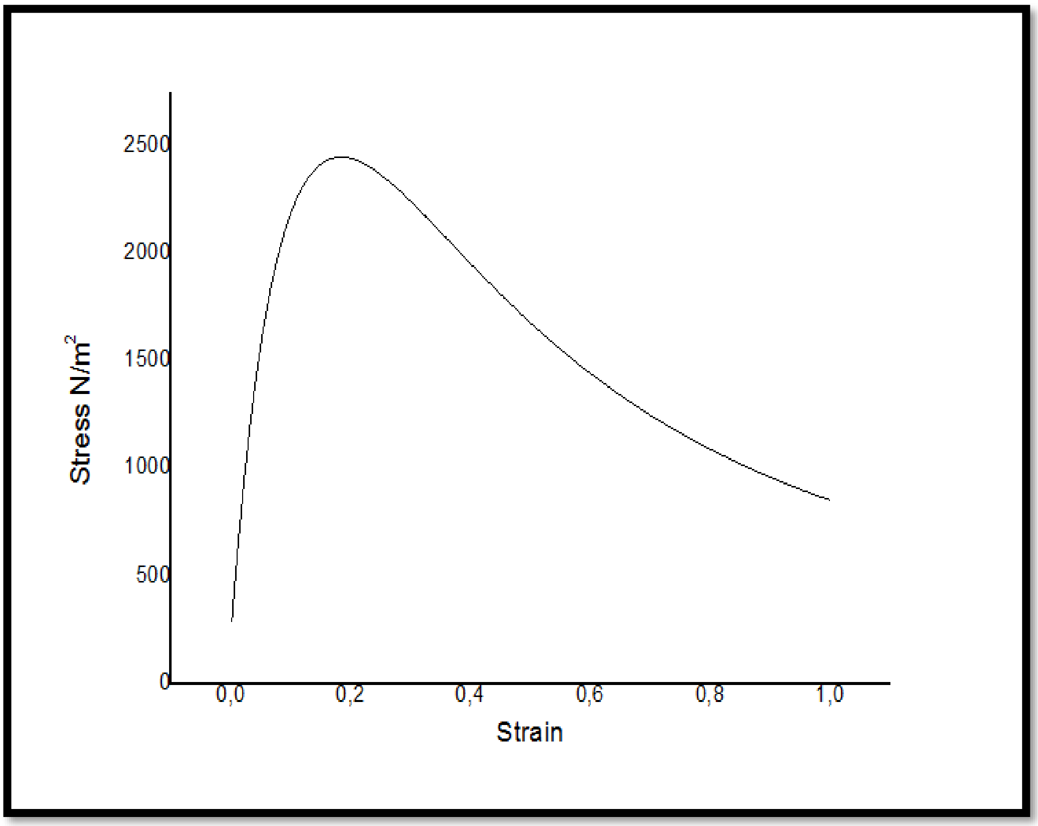


Figure 10. Stress Strain curve of a polyacrylamide.

We notice that curves are similar to those of the experiment. In fact, the stress-strain graph has different points or regions as follows:

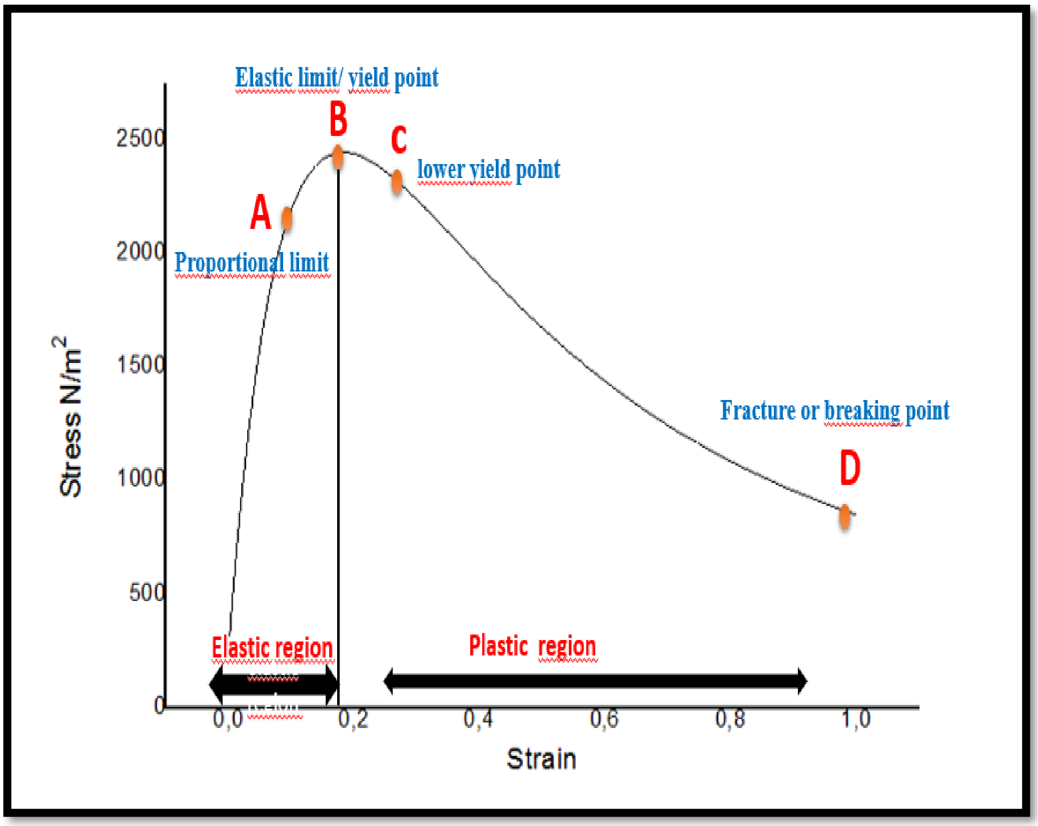


Figure11. Stress Strain curve of polyacrylamide.

A. Proportional limit
B. Elastic limit
C. Yield point
D. Fracture or breaking point

(A) Proportional limit

It is the region in the stress-strain curve that obeys Hooke's Law. In this limit, the ratio of stress with strain gives us proportionality constant known as young's modulus. The point A in the graph is called the proportional limit. So the polyacrylamide chain shows an elastic behavior.

(B) Elastic limit

It is the point in the graph up to which the polyacrylamide chain returns to it original position when the load acting on it is completely removed. Beyond this limit, the PAM chain doesn't return to its original position and a plastic deformation starts to appear in it.

(C) Yield point

The yield point is defined as the point at which the material starts to deform plastically. After the yield point is passed, permanent plastic deformation occurs. There are two yield points upper yield point and lower yield point.

(D) Fracture or breaking point

It is the point in the stress-strain curve at which the failure of the material takes place. On the curve of deformation the polyacrylamide has a breaking point.

7-Conclusion

In this chapter we can say that the modification of the dimensions of materials in response to mechanical forces is called deformation, we can also say that lammps plays a key role in our study because it allows us to study the deformation of materials as a function of stress, Avogadro software allows us to create the model of polyacrylamide and to calculate the energy of minimization, The stress-strain graph has different points or regions : Proportional limit , elastic limit ,yield point fracture or breaking point. In the curves of the variation of energy as a function of time ,we notice that the energy decreases with time ,we also notice that the curves are almost the same although we changed the cut of.

References

[1] «Avogadro,» [En ligne]. Available: https://avogadro.cc/.

[2] «LAMMPS Documentation,» 27 May 2021. [En ligne]. Available: https://docs.lammps.org/Manual.pdf.

[3] Mohammadreza Saboktakin, Advances in Chemistry Research, Nova publishers, January 2012.

[4] J. d. P. Peter Atkins, Physical Chemistry, New York: W. H. Freeman and Company, 2006.

[5] Xipeng Wang,Simòn Ramírez-Hinestrosa,Jure Dobnikar, and Daan Frenkela, «The Lennard-Jones potential: when (not) to use it,» *arxiv,* p. 14, 15 10 2019.

[6] SAMUEL J. LING, TRUMAN STATE UNIVERSITY ...all, university physics volume 1, Houston, Texas: openstax, 2016.

General conclusion

Molecular dynamics simulation is becoming a very powerful tool for studying dynamic phenomena in materials. The simulation yields information about interaction at length and time scales unattainable by experimental measurements and unpredictable by continuum theories. A very important characteristic of polymers is that their physical properties do not rely on the detailed chemical structure of the molecular chains but only on their flexibility, and accordingly they will be able to adopt different conformations. Polyacrylamide is a polymer used in many applications such as water treatment and pharmacy applications.

In this manuscript, a linear model based on acrylamide monomer is considered using Avogadro software, this system was geometrically optimized. To study the deformation of this model, the molecular dynamics program LAMMPS was used. This program has many commands that can be used to modeling and predict many properties especially mechanical properties, in this work, this program is used to modeling the deformation of the linear polyacrylamide.

LAMMPS executes by reading commands from an input script (text file), one line at a time. When the input script ends, LAMMPS exits. Each command causes LAMMPS to take some action. It may set an internal variable, read in a file, or run a simulation. Most commands have default settings.The output result shows that the energy is decreased in response to the time of the simulation. The stress-strain curve was obtained, showing many steps, the linear polyacrylamide present an elastic behavior with a limit « **Proportional limit** » *i*t is the region in the stress-strain curve that obeys Hooke's Law. In this limit, the ratio of stress with strain gives us proportionality constant known as young's modulus. So the polyacrylamide chain shows an elastic behavior. There is the **« Elastic limit »** it is the point in the graph up to which the polyacrylamide chain returns to it original position when the load acting on it is completely removed. Beyond this limit, the PAM chain doesn't return to its original position and a plastic deformation starts to appear in it. Then we have « **Yield point »** is defined as the point at which the material starts to deform plastically. After the yield point is passed, permanent plastic deformation occurs. There are two yield points upper yield point and lower yield point. Finaly « **Fracture or breaking point »** it is the point in the stress-strain curve at which the failure of the material takes place. On the curve of deformation the polyacrylamide has a breaking point. This theoretical result is compared with the allure of the experimental data, good coordination is noted.

ملخص

أصبحت محاكاة الديناميكيات الجزيئية أداة قوية جدًا لدراسة الظواهر الديناميكية في المواد ، وفي هذه المذكرة ، تم اعتبار نموذج خطي يعتمد على مادة الأكريلاميد باستخدام برنامج إفوقادرو ، وقد تم تحسين هذا النظام هندسيًا .لدراسة تشوه هذا النموذج ، تم استخدام برنامج الديناميكيات الجزيئية لامس .يحتوي هذا البرنامج على العديد من الأوامر التي يمكن استخدامها للنمذجة والتنبؤ بالعديد من الخصائص وخاصة الخصائص الميكانيكية ، و لهذا في هذا العمل ، تم استخدام هذا البرنامج لنمذجة تشوه بولي أكريلاميد الخطي

Abstract

Molecular dynamics simulation is becoming a very powerful tool for studying dynamic phenomena in materials.In this manuscript, a linear model based on acrylamide monomer is considered using Avogadro software, this system was geometrically optimized. To study the deformation of this model, the molecular dynamics program LAMMPS was used. This program has many commands that can be used to modeling and predict many properties especially mechanical properties, in this work, this program is used to modeling the deformation of the linear polyacrylamide.

Résumé

La simulation de dynamique moléculaire devient un outil très puissant pour étudier les phénomènes dynamiques dans les matériaux.Dans ce manuscrit, un modèle linéaire basé sur le monomère acrylamide est considéré en utilisant le logiciel Avogadro, ce système a été optimisé géométriquement. Pour étudier la déformation de ce modèle, le programme de dynamique moléculaire LAMMPS a été utilisé. Ce programme possède de nombreuses commandes qui peuvent être utilisées pour modéliser et prédire de nombreuses propriétés notamment mécaniques, dans ce travail, ce programme est utilisé pour modéliser la déformation du polyacrylamide linéaire.