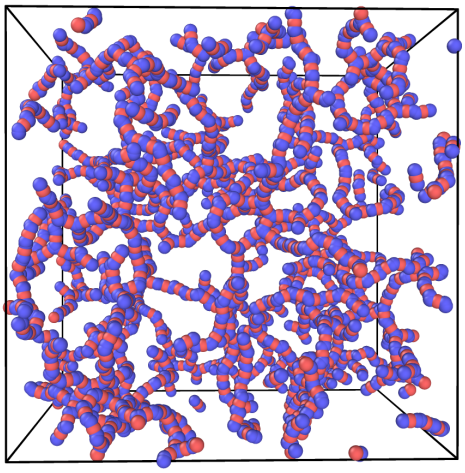
MTEK0033 Multiscale Modelling, University of Turku, January 2026

Brownian Dynamics Simulation

Project- IV



Created by: Vikki Anand Varma
Supervised by: Prof. Alberto Scacchi

If you come across any problems, please email at vavarm@utu.fi

Table of Contents

1 Tensile Deformation and Environmental Effects in Carbon Nanotubes

This project focuses on the **mechanical response of carbon nanotubes (CNTs)** subjected to **uniaxial tensile stress** using molecular dynamics simulations. One end of the CNT is held fixed, while the opposite end is pulled at a controlled rate. Students will investigate how bond breakability, temperature, and surrounding environment influence the elastic and failure properties of CNTs.

Carbon nanotubes are among the strongest known materials and are widely used in nanoelectronics, composite reinforcements, sensors, and biomedical applications. Understanding how CNTs deform and fail under tensile loading, particularly in realistic environments, is essential for reliable nanodevice design.

1.1 Introduction

Carbon nanotubes exhibit extraordinary mechanical properties, including Young's modulus exceeding 1 TPa and tensile strength on the order of 100 GPa. However, these properties depend sensitively on loading conditions, temperature, defects, and the surrounding medium.

In realistic operating conditions, CNTs often experience uniaxial tension rather than idealized loading. Thermal fluctuations, bond rupture, and interactions with surrounding fluids can significantly alter the stress-strain response and failure mechanisms.

In this project, students will study CNT deformation under tensile loading considering:

- Unbreakable (harmonic or Tersoff-style) bonds
- Dry (vacuum) and water-immersed environments

1.2 Simulation Model

1.2.1 Carbon Nanotube Geometry

A single-wall armchair carbon nanotube of chirality $(10, 10)$ is used throughout the project.

- Length: $L = 20$ nm
- Diameter: $d \approx 1.36$ nm
- Number of carbon atoms: ~ 1600

1.2.2 Interatomic Potentials

Two bonding scenarios are considered:

- **Unbreakable bonds**: Tersoff or AIREBO potential with bond breaking disabled

- **Breakable bonds**: AIREBO or REBO potential allowing bond rupture

1.2.3 Water Environment

For immersed simulations, the CNT is placed in explicit water modeled using the SPC/E or TIP3P model. Carbon–water interactions are described using Lennard–Jones potentials.

1.3 Tensile Deformation Protocol

Uniaxial tension is applied by fixing one end of the CNT and pulling the opposite end along the tube axis at a constant velocity v.

$$\epsilon(t) = \frac{L(t) - L_0}{L_0}, \tag{1}$$

where ϵ is the tensile strain, L_0 is the initial tube length, and $L(t)$ is the instantaneous length.

The tensile stress is computed from the axial virial stress:

$$\sigma = \frac{F}{A}, \tag{2}$$

where F is the measured axial force and $A = \pi d t$ is the effective cross-sectional area, with wall thickness $t = 0.34$ nm.

1.4 Symbols

Symbol	Meaning	Unit
σ	tensile stress	GPa
ϵ	tensile strain	–
E	Young's modulus	GPa
T	temperature	K
L	CNT length	nm
d	CNT diameter	nm
$\dot{\epsilon}$	strain rate	ps^{-1}

Table 1: List of symbols used in the project.

1.5 Project Tasks

- Build a single-wall CNT with correct chirality
- Fix one end and apply uniaxial tensile loading to the other end
- Compute stress–strain curves
- Extract Young's modulus from the linear regime
- Identify yield, fracture strain, and failure stress

- Compare breakable vs unbreakable bonds
- Study temperature and environmental effects

1.6 Simulation Studies

Study 1: Tensile Response of a Dry CNT (Unbreakable Bonds)
In this study, you will investigate the tensile response of a single, dry carbon nanotube (CNT) subjected to uniaxial stretching. The CNT bonds are treated as unbreakable, allowing you to focus on elastic deformation and temperature-dependent mechanical response without complications from fracture. The primary quantities of interest are the stress–strain relationship, Young's modulus, and the effect of temperature on elastic behavior.

#	Temperature (K)
1	100
2	300
3	500
4	700

Table 2: Temperatures used to study the tensile response of a dry CNT with unbreakable bonds.

Step 1: Folder structure and setup

1. Navigate to the main project directory:

   `Project_4/CNT_Tensile_Test/`

2. Inside this directory, you will find four subfolders corresponding to the temperatures listed in Table 1:

   `T_100K`, `T_300K`, `T_500K`, `T_700K`

3. Each folder contains:
   - the LAMMPS input script for tensile deformation,
   - the CNT structure and data files,
   - potential files with unbreakable bonds,
   - and Python scripts for post-processing stress–strain data.

Step 2: CNT and simulation parameters

1. The CNT geometry (chirality, length, and diameter) is fixed for all simulations.
2. Bond breaking is disabled; all C–C bonds remain intact throughout the deformation.
3. The system is simulated in vacuum (dry CNT), with no surrounding fluid or matrix.

4. The system temperature is controlled using a thermostat and set according to the folder name.

Step 3: Tensile deformation protocol

1. Apply uniaxial tensile deformation along the CNT axis using a constant engineering strain rate.
2. The strain is increased gradually to ensure quasi-static deformation.
3. During deformation, the axial stress and strain are recorded in the log file and/or output data files.

Step 4: Running the simulations

1. For each temperature folder, run the LAMMPS input script until the target maximum strain is reached.
2. Ensure that the system remains stable and no numerical instabilities occur.
3. The stress–strain data are saved automatically during the simulation.

Step 5: Data analysis

1. Use the provided Python scripts to plot stress as a function of strain for each temperature.
2. From the linear elastic regime, extract Young's modulus.
3. Compare stress–strain curves at different temperatures.

Step 6: Physical interpretation

1. Discuss how temperature affects the elastic response of the CNT.
2. Explain why Young's modulus may decrease with increasing temperature.
3. Comment on the limitations of using unbreakable bonds when modeling real CNTs.

Study 2: Effect of Strain Rate on CNT Tensile Response

In this study, you will investigate how the applied strain rate influences the tensile response of a dry carbon nanotube (CNT). All system parameters, including CNT geometry, interaction potentials, and temperature, are kept fixed. Only the applied engineering strain rate $\dot{\epsilon}$ is varied. The primary objective is to understand rate-dependent mechanical behavior and identify deviations from quasi-static deformation.

#	$\dot{\epsilon}$ (ps^{-1})
1	1×10^{-4}
2	5×10^{-4}
3	1×10^{-3}

Table 3: Strain rates used to study rate-dependent tensile deformation of a CNT.

Step 1: Folder structure and setup

1. Navigate to the directory:

   `Project_4/CNT_Tensile_Test/Strain_Rate/`

2. Inside this directory, you will find three subfolders corresponding to the strain rates listed in Table 1:

   `SR_1e-4`, `SR_5e-4`, `SR_1e-3`

3. Each folder contains:

   - the LAMMPS input script with the specified strain rate,
   - the CNT structure and data files,
   - potential files (unbreakable bonds),
   - and post-processing scripts for stress–strain analysis.

Step 2: Simulation parameters

1. The CNT geometry and bond parameters are identical for all simulations.
2. The temperature is fixed (e.g., $T = 300$ K) across all strain-rate studies.
3. Only the applied engineering strain rate $\dot{\epsilon}$ differs between folders.
4. Ensure that the thermostat and deformation protocol are consistent in all runs.

Step 3: Tensile deformation protocol

1. Apply uniaxial tensile deformation along the CNT axis using the specified strain rate.
2. Record the axial stress and strain throughout the deformation.
3. Run each simulation until the same maximum strain is reached.

Step 4: Data analysis

1. Plot stress–strain curves for all strain rates on the same graph.
2. Identify differences in slope, stress fluctuations, and non-linear response.
3. Determine whether the response remains quasi-static at lower strain rates.

Step 5: Physical interpretation

1. Explain why higher strain rates can lead to increased apparent stiffness or stress overshoot.
2. Discuss the role of atomic relaxation times in rate-dependent deformation.
3. Comment on the limitations of molecular dynamics when probing experimentally realistic strain rates.

Study 3: Tensile Response of a CNT in Water (Unbreakable Bonds)

In this study, you will examine how a surrounding aqueous environment influences the tensile response of a carbon nanotube (CNT). The CNT bonds are treated as unbreakable, allowing you to isolate environmental effects such as thermal fluctuations, viscous damping, and CNT–water interactions. The primary goal is to compare the elastic response of a CNT in water with that of a dry CNT at different temperatures.

#	Temperature (K)
1	300
2	350
3	400
4	500

Table 4: Temperatures used to study the effect of water on CNT elasticity.

Step 1: Folder structure and setup

1. Navigate to the directory:

   `Project_4/CNT_Tensile_Test/CNT_in_Water/`

2. Inside this directory, you will find three subfolders corresponding to the temperatures listed in Table 1:

   `T_300K`, `T_350K`, `T_400K`

3. Each folder contains:

   - the LAMMPS input script for tensile deformation,
   - the CNT structure and topology files,
   - water molecule definitions and force-field files,
   - and post-processing scripts for stress–strain analysis.

Step 2: System and simulation parameters

1. The CNT geometry and bond parameters are identical to those used in the dry CNT studies.
2. Bond breaking is disabled; all C–C bonds remain intact during deformation.
3. The CNT is fully immersed in water, with periodic boundary conditions applied in all directions.
4. The system temperature is controlled using a thermostat and set according to the folder name.

Step 3: Equilibration protocol

1. First equilibrate the CNT–water system without deformation to ensure thermal and mechanical equilibrium.
2. Allow sufficient time for the water molecules to relax around the CNT surface.
3. Verify that temperature and pressure have stabilized before applying tensile strain.

Step 4: Tensile deformation

1. Apply uniaxial tensile deformation along the CNT axis using the same strain rate as in the dry CNT study.
2. Record axial stress and strain throughout the deformation process.
3. Run each simulation up to the same maximum strain for all temperatures.

Step 5: Data analysis

1. Plot stress–strain curves for all temperatures.
2. Extract Young's modulus from the linear elastic regime.
3. Compare the elastic response of the CNT in water with that of the dry CNT at the same temperature.

Step 6: Physical interpretation

1. Discuss how water influences thermal fluctuations and stress transmission in the CNT.
2. Explain the role of viscous damping and CNT–water interactions in modifying the mechanical response.
3. Comment on why elastic properties in water may differ from those in vacuum.

Study 4: Comparison of Mechanical Properties
Students will compare Young's modulus, tensile strength, and fracture strain across all scenarios and discuss environmental softening or strengthening effects.

1.7 Expected Observables

- Stress-strain curves
- Young's modulus E (GPa)
- Fracture strain and tensile strength
- Bond rupture statistics and spatial maps

1.8 Presentation and Project Report

- **Introduction (1 page)**: Polymer translocation in biological and synthetic systems
- **Model and Theory (1 page)**: Brownian dynamics, non-additivity, entropic barriers
- **Results and Discussion (6–10 pages)**: Scaling, distributions, driving mechanisms
- **Conclusion (1 page)**: Physical interpretation and limitations

1.9 Future aspects

Write about possible extensions and future aspects including defected CNTs, multi-wall nanotubes, cyclic loading, chemical functionalization, fracture toughness analysis, and coupling to continuum elasticity models.

2 Project Report Guidelines

1. Introduction to the Problem

This section should be approximately one page long (or slightly more) and must include at least five (minimum three) scientific references from peer-reviewed literature.
The introduction should present an overview of carbon nanotubes (CNTs) as advanced nanomaterials and discuss their exceptional mechanical properties. In particular, students should:

- Introduce the structure of carbon nanotubes and their bonding characteristics.
- Explain why CNTs exhibit high stiffness, strength, and fracture resistance.
- Briefly describe stress–strain behavior in crystalline solids.
- Introduce the concepts of elastic modulus, yield point, and failure strain.

Students should also motivate the relevance of CNT mechanics by discussing applications such as:

- Nano-electromechanical systems (NEMS),
- Reinforcement in composite materials,
- Biomedical and sensing applications.

The goal of the project should be clearly stated:

To investigate how temperature, strain rate, and environment influence the tensile response of carbon nanotubes.

2. Technical Description of the Simulations

This section should describe the molecular dynamics framework used to study CNT deformation. Students must describe:

- The interatomic potential used for carbon–carbon interactions.
- The meaning of unbreakable bonds and their role in isolating elastic behavior.
- Boundary conditions applied along the tensile direction.
- The ensemble used during deformation (e.g., NVT or NVE).

The method used to apply tensile strain should be clearly explained, including how strain and stress are measured during the simulation.

3. Study 1: Temperature Dependence of Tensile Response (Dry CNT)

In this study, students will analyze how temperature affects the elastic response of a dry CNT with unbreakable bonds.

Procedure

- Perform tensile simulations at multiple temperatures.
- Record stress–strain curves for each temperature.
- Ensure that the strain rate is kept constant across all simulations.

Analysis

Students should:

- Plot stress–strain curves at different temperatures on the same graph.
- Extract the Young's modulus from the linear elastic regime.
- Discuss how thermal fluctuations influence stiffness and failure strain.

4. Study 2: Effect of Strain Rate

In this study, students will examine how the applied strain rate influences the tensile response of the CNT.

Procedure

- Perform tensile simulations at different strain rates.
- Keep temperature and CNT geometry fixed.
- Record stress–strain data for each strain rate.

Analysis

Students should:

- Compare stress–strain curves obtained at different strain rates.
- Discuss viscoelastic and rate-dependent effects in atomistic systems.
- Explain why higher strain rates can lead to apparent stiffening.

5. Study 3: Environmental Effects — CNT in Water

In this study, students will explore how a surrounding solvent modifies the mechanical response of a CNT.

Procedure

- Embed the CNT in an explicit water environment.
- Perform tensile simulations at different temperatures.
- Ensure that CNT bonds remain unbreakable to isolate environmental effects.

Analysis

Students should:

- Compare stress–strain curves for dry and solvated CNTs.
- Discuss how water molecules influence stress transfer and damping.
- Comment on thermal and hydrodynamic effects introduced by the solvent.

6. Main Findings and Discussion

This section should form the core of the report and be approximately 5–10 pages long (or 3–6 pages for a shorter report).
Students should integrate results from all three studies and discuss:

- The combined effects of temperature, strain rate, and environment.
- The physical mechanisms underlying observed trends.
- The limitations of unbreakable-bond models in predicting failure.

Connections to continuum elasticity theory and nanoscale mechanics should be made wherever appropriate.

7. Conclusion

This section should be approximately half a page to one page long.
The conclusion should:

- Summarize the key mechanical trends observed in CNT deformation.
- Highlight the role of molecular dynamics in nanoscale mechanics.
- Reflect on how environmental and loading conditions influence CNT performance.
- Suggest possible extensions, such as bond breaking, defects, or multi-walled CNTs.

References

[1] Li, Jian, et al. **"Mechanical and thermal properties of graphyne-coated carbon nanotubes: a molecular dynamics simulation on one-dimensional all-carbon van der Waals heterostructures."** Physical Chemistry Chemical Physics 25.12 (2023): 8651-8663.

[2] **Computer Simulation of Liquids** by Allen and Tildesley.

[3] **Theory of Simple liquids** by Hansen and McDonald.

[4] **Nonequilibrium Statistical Mechanics** by Robert Zwanzig