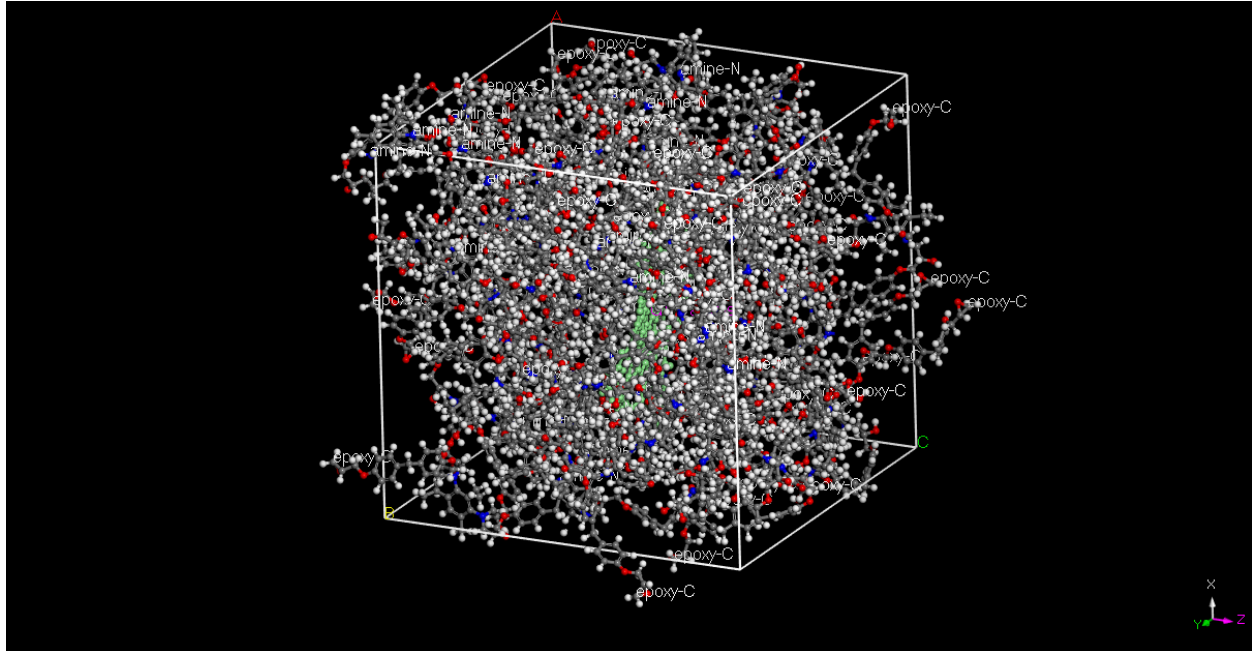




Molecular modelling to investigate material properties of graphene nanoplatelet composites

Calculating elastic properties of a graphene nanoplatelet/epoxy composite with molecular dynamics using BIOVIA Materials Studio and COMPASS force field

Master's thesis in Applied Mechanics

MARCUS PETERSSON

DEPARTMENT OF INDUSTRIAL AND MATERIALS SCIENCE

CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2026
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MASTER'S THESIS 2026

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Cover: Graphene nanoplatelet in green surrounded by cross-linked epoxy molecules

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Abstract

This master's thesis investigates the molecular modelling of material properties of graphene nanoplatelet (GNP)/epoxy composites using molecular dynamics (MD) simulations. A cross-linked epoxy matrix (DGEBF/DETDA) with embedded GNPs was constructed in BIOVIA Materials Studio using the COMPASS force field. Elastic constants were calculated via the strain fluctuation method, yielding full compliance tensors and derived Young's moduli. Results from production runs lasting 50 ps and 100 ps were compared, showing that simulation length substantially affects predicted values, with relative errors in compliance components sometimes exceeding the mean values. While Young's moduli (approximately 1.6–2.6 GPa) were of the same order of magnitude as experimental references (≈ 3 GPa at 3–4 wt% GNP), the high statistical errors highlight the need for convergence studies. Additional contributions include the development of a workflow for molecular modelling with MD and the finding that MD simulations of insufficient duration limit the accuracy of the modelling. The thesis concludes with recommendations for longer simulations and the use of high-performance computing platforms (e.g. LAMMPS or GROMACS), as well as future work on neural network surrogate models for investigating plastic material behaviour.

Keywords: Molecular dynamics, graphene nanoplatelets, polymer nanocomposites, strain fluctuation, elasticity, material modelling

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Marcus Petersson, Gothenburg, June 2026

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1

Introduction

1.1 Background

Composite materials are increasingly used in industries because they can be both lightweight and strong [1]. Nanocomposite materials are a type of composite material, in which the dimensions of the filler are in the nanometre range. Incorporating nanofillers into a polymer matrix can substantially enhance electrical conductivity and mechanical properties compared with the neat matrix, even at low weight percentages. The nanoscale size of the fillers leads to a very high specific surface area and a large interfacial region with the matrix, which can strengthen filler-matrix interactions and improve load transfer and electrical conductivity [2, 3].

One type of nanofiller is graphene nanoplatelets (GNPs). GNPs are thin plates of a few layers of graphene, which results in a high surface-to-volume ratio, allowing each platelet to interact with a large volume of the surrounding material. They are also easy and inexpensive to manufacture compared to other nanoscale carbon fillers, which, together with the natural abundance of graphite (which graphene is made of), makes GNP composites a suitable material choice [4]. Examples of applications of the material are found in strain sensors for structural health monitoring [5], supercapacitors [6] and improvement techniques of the electro-mechanical performance of solar cells [7]. Figure 1.1 shows a GNP with six layers of graphene. The macroscale mechanical behaviour of GNP composites is greatly influenced by atomic-level interfacial effects between the GNP and the matrix [8].

Molecular dynamics is a numerical method for solving the equations of motion for systems of many atoms. It is used for atomistic material modelling. This thesis aims to calculate the material parameters of a GNP/epoxy composite with molecular dynamics simulations and to provide a framework for atomic-level material modelling of such a material. In particular, the elastic material parameters will be calculated to investigate the concept and to develop the basic framework for the modelling of the material.

1.2 Aim

The aim of this project is to calculate elastic material parameters of a GNP/epoxy composite, where the epoxy consists of diglycidyl ether of bisphenol F (DGEBF or EPON-862) and diethyltoluenediamine (DETDA). The predicted elastic parameters will be compared with experimentally determined values, with the purpose to analyse the validity of the method to model the mechanical behaviour of the material.

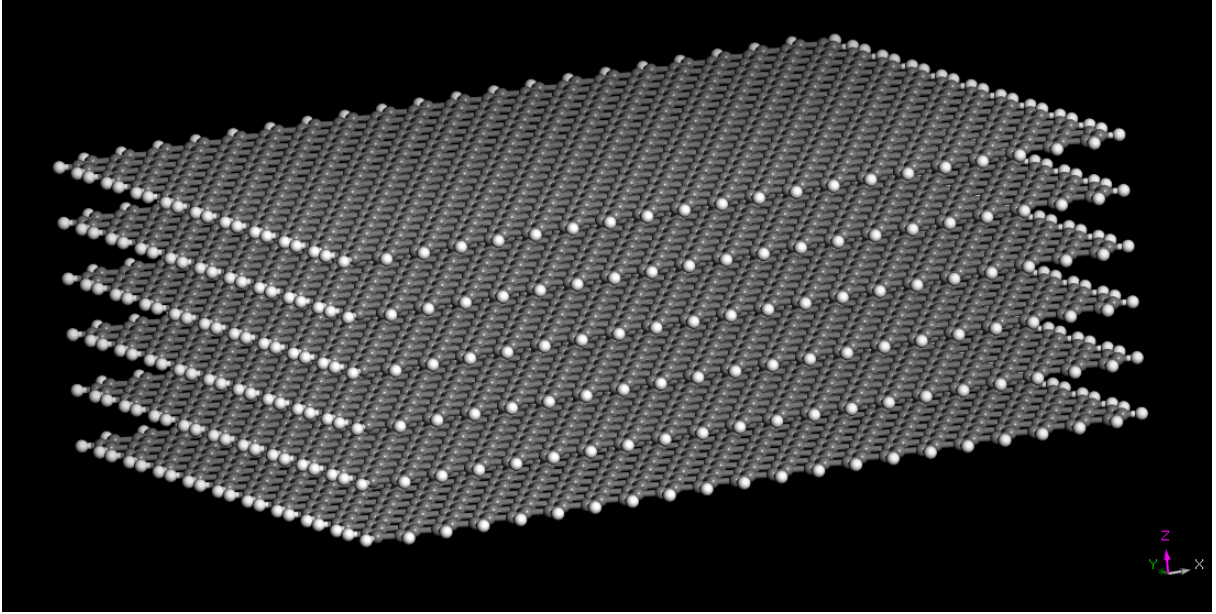


Figure 1.1: *Six layers of hydrogen-terminated graphene forming a GNP illustrated in the Materials Visualizer in BIOVIA Materials Studio.*

1.3 Limitations

As mentioned, the study is only focused on elastic material behaviour. Additionally, the GNP studied only consisted of one layer of graphene. The MD simulations were done on an HP ZBook Fury 16 G9 Mobile Workstation PC with 128 GB RAM and 24 cores of the model 12th Gen Intel(R) Core(TM) i7-12850HX. The software used for the MD simulations was BIOVIA Materials Studio which is not supported to run on the Chalmers computer cluster, which resulted in having to do shorter MD simulations.

2

Theory

2.1 Molecular dynamics

Molecular dynamics (MD) is a simulation method that numerically solves Newton's second equation

$$F_i^{(\alpha)} = m^{(\alpha)} \ddot{r}_i^{(\alpha)} \quad (2.1)$$

for a system of atoms $\alpha = 1, \dots, N$, where

$$F_i^{(\alpha)} = -\frac{\partial U}{\partial r_i^{(\alpha)}}, \quad (2.2)$$

U is the potential energy and $r_i^{(\alpha)}$ is the position of particle α in the i -direction. The choice of the potential energy function affects the simulation results; for example bond stiffnesses and strengths affect mechanical property results.

2.1.1 Force fields

The force field or potential energy function used for an MD simulation can differ depending on what type of material is analysed. The most basic force field is the 12-6 Lennard-Jones potential. For a pair of particles at a distance r from each other, it is formulated as

$$U_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (2.3)$$

where ε is the depth of the potential well and σ is the distance between the particles that results in zero potential energy. The Lennard-Jones potential only accounts for van der Waals forces, so other more detailed force fields have been developed for a more comprehensive description of the interatomic forces, including contributions from bond lengths and angles as well as torsions of molecules. One example of such a force field is the COMPASS force field. COMPASS is an acronym that stands for Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies and it is a so-called consistent force field. The functional form of a consistent force field is

$$U = U_{bond} + U_{angle} + U_{torsion} + U_{oop} + U_{cross} + U_{non-bond}. \quad (2.4)$$

The energies U_{bond} , U_{angle} , $U_{torsion}$, U_{oop} , U_{cross} and $U_{non-bond}$ are associated with bond length, bond angle, bond torsion, out-of-plane interactions, cross-terms between the other bond interactions and non-bond related energies such as electrostatic and van der Waals interactions respectively [9, p. 2].

2.1.2 Equilibration

An MD simulation is usually done by first equilibrating the simulation box with constant NVT and/or NPT, where N is the number of particles, T is the temperature, V is the volume and P is the pressure. The temperature and the pressure are controlled by a thermostat and a barostat respectively. There are several different methods to control the temperature and pressure and the choice of method affects the simulation results. Some examples are the Nosé-Hoover thermostat and the Parrinello-Rahman barostat.

2.1.2.1 Nosé-Hoover thermostat

The Nosé-Hoover thermostat controls the particle velocities, i.e. the temperature, by adding a friction-like term to the system. The Hamiltonian then becomes

$$H = \sum_{\alpha=1}^N \frac{1}{2m^{(\alpha)}} p_i^{(\alpha)} p_i^{(\alpha)} + \phi(\mathbf{r}) + \frac{1}{2} Q \zeta^2 + N_f k_B T_0 \ln S, \quad (2.5)$$

where $p_i^{(\alpha)}$ is the momentum of particle α in the i -direction, N_f is the number of degrees of freedom, k_B is the Boltzmann constant and T_0 is the target temperature. ζ and $\ln S$ are fictitious variables associated with the extra degree of freedom from the interaction between the structure and the heat bath and act as velocity and position variables respectively, where the associated mass is Q [10]. From the Hamiltonian, the equations of motion for the Nosé-Hoover thermostat can be derived.

2.1.2.2 Parrinello-Rahman barostat

The Parrinello-Rahman barostat controls the pressure by adjusting the cell parameters. It is done by decomposing the coordinate vector in index notation like

$$r_i^{(\alpha)} = h_{ij} s_j^{(\alpha)}, \quad (2.6)$$

where

$$\mathbf{h} = [\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}] \quad (2.7)$$

and $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are the cell basis vectors (column vectors), while $s_j^{(\alpha)}$ represents the fractional coordinates of particle $\alpha = 1, \dots, N$. A system of two coupled equations (2.8) then arises

$$\begin{cases} F_i^{(\alpha)} - m^{(\alpha)} \dot{h}_{ij} h_{jk}^{-1} \dot{r}_k^{(\alpha)} = m^{(\alpha)} \ddot{r}_i^{(\alpha)}, \\ W \ddot{h}_{ij} = V \left(P_{ik}^{(int)} - P_{ik}^{(ext)} \right) h_{kj}^{-T}. \end{cases} \quad (2.8)$$

Here $V = \det(\mathbf{h})$ is the cell volume and $P_{ik}^{(ext)}$ is the target pressure tensor and the cell's internal pressure tensor is

$$P_{ij}^{(int)} = \frac{1}{V} \left[\sum_{\alpha=1}^N m^{(\alpha)} \dot{r}_i^{(\alpha)} \dot{r}_j^{(\alpha)} - \sum_{\alpha=1}^N r_i^{(\alpha)} \frac{\partial U}{\partial r_j^{(\alpha)}} \right]. \quad (2.9)$$

W is a non-physical barostat parameter with the dimension of mass, which can be chosen on the basis of computational convenience, and it determines the inertia governing the system's response to a difference between the reference pressure and the current pressure [11, p. 7184].

A version of the Parrinello-Rahman barostat that is used in Materials Studio for pressure control is called the Martyna-Tobias-Klein (MTK) barostat, which was developed to correctly sample the isobaric-isothermic ensemble and thus makes it appropriate for production MD simulations in that ensemble [12]. The Hamiltonian for the MTK barostat is

$$H = \frac{1}{2} \sum_{\alpha=1}^N m^{(\alpha)} \dot{s}_i^{(\alpha)} G_{ij} \dot{s}_j^{(\alpha)} + \sum_{\alpha=1}^{N-1} \sum_{\beta=\alpha+1}^N \phi(\mathbf{r}_\alpha - \mathbf{r}_\beta) + \frac{1}{2} Q \text{Tr} \left(h_{ij}^{-1} \dot{h}_{jk}^T \dot{h}_{kl} h_{lm}^{-1} \right) + p_0 V, \quad (2.10)$$

where m denotes the particle mass, $G_{ij} = h_{ik}^T h_{kj}$, ϕ is the interatomic potential function, Q is a volume change inertia parameter (similar to W in equation (2.8)) and p_0 is the target pressure [10]. The α and β superscripts denote particle indices. The equations of motion can be derived from the Hamiltonian.

2.1.2.3 Berendsen barostat

The Berendsen barostat regulates the pressure by only scaling the volume of the simulation cell. For each time step equation (2.1) is solved for all the atoms and the volume is scaled as

$$V_{n+1} = V_n \left[1 + \frac{\Delta t}{\tau_P} \beta_T (P_n - P_0) \right], \quad (2.11)$$

where τ_P is the pressure coupling time constant and β_T is the isothermal compressibility. The Berendsen barostat does not, however, correctly sample the isobaric-isothermic ensemble if used in NPT simulations and is better used only for reaching equilibrium [13].

2.1.3 Production

After the system has been equilibrated and the initial positions and velocities have been set, the equations of motion can be solved for all particles. A common algorithm used to solve the system of ODEs is the Velocity-Verlet algorithm. The algorithm consists of the following steps:

$$\begin{aligned} &\text{Calculate } v_i^{(\alpha)} \left(t + \frac{1}{2} \Delta t \right) = v_i^{(\alpha)}(t) + \frac{1}{2} a_i^{(\alpha)}(t) \Delta t \\ &\text{Calculate } r_i^{(\alpha)}(t + \Delta t) = r_i^{(\alpha)}(t) + v_i^{(\alpha)} \left(t + \frac{1}{2} \Delta t \right) \Delta t \\ &\text{Use } a_i^{(\alpha)}(t + \Delta t) = \frac{1}{m} F_i(\mathbf{r}^{(\alpha)}(t + \Delta t)) \\ &\text{Calculate } v_i^{(\alpha)}(t + \Delta t) = v_i^{(\alpha)} \left(t + \frac{1}{2} \Delta t \right) + \frac{1}{2} a_i^{(\alpha)}(t + \Delta t) \Delta t \end{aligned} \quad (2.12)$$

for particle α , where $F_i(\mathbf{r})$ is derived from the potential energy function [14, pp. 648–649]. By using an appropriate ensemble, the resulting $r_i(t)$, $v_i(t)$ and $a_i(t)$ can be used to calculate properties of the analysed system, such as heat capacity [15] or static structure factor [16]. To calculate elastic material parameters an isobaric-isothermic ensemble could for example be used to let the simulation cell volume fluctuate.

2.1.4 Error estimation

It is of interest to estimate the statistical uncertainty of results from MD simulations. Let A be an averaged property that is calculated from values at each time step of the MD

simulation as

$$A = \langle \mathcal{A} \rangle = \frac{1}{M} \sum_{i=1}^M \mathcal{A}_i. \quad (2.13)$$

The estimated error of A will render the expression

$$A = \langle \mathcal{A} \rangle \pm \sigma(A) \quad (2.14)$$

where $\sigma(A)$ is the standard deviation of A and M_{eff} is the number of correlated data points. If $\mathcal{A}_i$ were uncorrelated data points, the result would be calculated as

$$\text{Var}(\mathcal{A}) = \sigma^2(\mathcal{A}) = \langle \mathcal{A}^2 \rangle - \langle \mathcal{A} \rangle^2. \Rightarrow \text{Var}(A) = \frac{1}{M} \text{Var}(\mathcal{A}). \quad (2.15)$$

However, MD simulation data is often highly correlated since the data points depend on the previous time step. By introducing the statistical inefficiency s , it can be analysed how correlated the data is and thereby how $\text{Var}(A)$ relates to $\text{Var}(\mathcal{A})$. The number of correlated data points is

$$M_{\text{eff}} = \frac{M}{s}, \quad (2.16)$$

where M is the total number of time steps in the simulation. When the data is correlated, the variance of the original calculated averaged property A is then calculated as

$$\text{Var}(A) = \frac{1}{M_{\text{eff}}} \text{Var}(\mathcal{A}) = \frac{s}{M} \text{Var}(\mathcal{A}). \quad (2.17)$$

The task is therefore to determine s , which can be done by first calculating the correlation function

$$\Phi_k = \frac{\langle \mathcal{A}_i \mathcal{A}_{i+k} \rangle - \langle \mathcal{A} \rangle^2}{\langle \mathcal{A}^2 \rangle - \langle \mathcal{A} \rangle^2}, \quad (2.18)$$

with the assumption of a stationary system, which implies that $\Phi_k = \Phi_{-k}$. It is deduced that $\Phi_k \rightarrow 0$ for large k . Next, a cut-off value M_c is defined, for which $\Phi_k \approx 0$ for $k > M_c$, but that still fulfils $M \gg M_c$. The variance of A can now be rewritten as

$$\begin{aligned} \text{Var}(A) &= \left\langle \left(\frac{1}{M} \sum_{i=1}^M \mathcal{A}_i - \langle \mathcal{A} \rangle \right)^2 \right\rangle \\ &= \frac{1}{M^2} \sum_{i=1}^M \sum_{j=1}^M [\langle \mathcal{A}_i \mathcal{A}_j \rangle - \langle \mathcal{A} \rangle^2] \end{aligned} \quad (2.19)$$

Stationarity implies that $\text{Cov}(\mathcal{A}_i, \mathcal{A}_j)$ is only dependent on the lag $k := i - j$. A function c can then be defined as

$$c(k) := \text{Cov}(\mathcal{A}_i, \mathcal{A}_{i+k}). \Rightarrow \text{Var}(A) = \frac{1}{M^2} \sum_{i=1}^M \sum_{j=1}^M c(j-i). \quad (2.20)$$

Since the summand depends only on the lag, the sum can be calculated over the lag. However, each pair (i, j) that maps to k must fulfil $i \in [1, M-k]$ for $k \geq 0$ and $i \in [1-k, M]$ for $k < 0$. Also the minimum and maximum values of k are for $(i, j) = (1, M)$ and $(i, j) = (M, 1)$ respectively, which means $k \in [-(M-1), M-1]$. There are $M - |k|$ terms for every i , which implies that

$$\sum_{i=1}^M \sum_{j=1}^M c(j-i) = \sum_{k=-(M-1)}^{M-1} \sum_{i=\max(1, 1-k)}^{\min(M, M-k)} c(k) = \sum_{k=-(M-1)}^{M-1} (M - |k|) c(k). \quad (2.21)$$

By using equation (2.18), it is deduced that

$$\text{Var}(A) = \text{Var}(\mathcal{A}) \frac{1}{M^2} \sum_{k=-(M-1)}^{M-1} (M - |k|) \Phi_k. \quad (2.22)$$

Now with (2.17)

$$\frac{s}{M} = \frac{1}{M^2} \sum_{k=-(M-1)}^{M-1} (M - |k|) \Phi_k. \Leftrightarrow s = \sum_{k=-(M-1)}^{M-1} \left(1 - \frac{|k|}{M}\right) \Phi_k. \quad (2.23)$$

Using that $\Phi_k \approx 0$ for $k > M_c$ and that $M_c \ll M \Rightarrow \frac{|k|}{M} \approx 0$ for $k < M_c$, the final expression for the statistical inefficiency can be written as

$$s = 1 + \sum_{k=1}^M \Phi_k. \quad (2.24)$$

The calculated value of s is then used with equation (2.17) to determine the error bounds for A .

2.2 Linear elasticity

As mentioned, MD simulations can be used to determine material parameters. In particular, when simulating small fluctuations of the cell, the linear elastic parameters of a material can be inferred. Linear elasticity describes the mechanical response of solids subjected to small deformations. Assuming infinitesimal strains, the relationship between stress and strain is linear and reversible, meaning that the material returns to its original configuration after the load is removed.

The motion of a deformable body is governed by the Cauchy momentum equation

$$\frac{\partial \sigma_{ij}}{\partial x_j} + f_i = \rho \ddot{u}_i \quad (2.25)$$

where σ_{ij} is the Cauchy stress tensor, f_i is the body force per unit volume, ρ is the material density, and u_i is the displacement field.

For small deformations, the infinitesimal strain tensor is defined as

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (2.26)$$

The strain tensor measures local changes in shape and volume of the material resulting from the displacement field.

In linear elasticity, stress and strain are related through Hooke's law

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}, \quad (2.27)$$

where C_{ijkl} is the fourth-order stiffness tensor. The components of the stiffness tensor describe the resistance of the material to deformation and fully characterise the elastic response of the material.

For anisotropic materials, the stress-strain relationship is commonly expressed using Voigt notation, where the stress and strain tensors are represented as six-component vectors. Hooke's law can then be written in matrix form as

$$\underline{\sigma} = [C]\underline{\varepsilon}, \quad (2.28)$$

where $[C]$ is the 6×6 stiffness matrix. The inverse of the stiffness matrix is known as the compliance matrix,

$$[S] = [C]^{-1}. \quad (2.29)$$

3

Methods

The MD simulations were performed using BIOVIA Materials Studio (MS), which has an application programming interface (API) that makes it possible to control the software and automate simulations by scripts in the Perl programming language. The commercial MS software was used because it enabled the simulations to be performed with a COMPASS force field which can provide accurate predictions of mechanical properties [17]. MS includes a module for molecular mechanics calculations called Forcite, which approximates the potential energy surface with a classical force field, and was developed using parameters derived from experimental studies [10].

3.1 Preparing simulation cell

The matrix of the composite was considered to be made of epoxy consisting of the resin diglycidyl ether of bisphenol F (DGEBF or EPON-862) and the hardener diethyltoluenediamine (DETDA). The structures of these molecules were imported from PubChem, a database for chemical information [18], after which the molecule bond angles were optimised with Forcite geometry optimisation. DGEBF and DETDA, which are shown in Figures 3.1a and 3.1b, were chosen because the polymer in the composite used in the mechanical property experiments in [19] consists of those substances.

The GNP was then constructed by importing the `Graphene.xsd` document which was included in the MS software download. The file consisted of only one hexagon of graphene (see Figure 3.2) in a periodic cell. To turn it into a plate, the

`Build → Symmetry → Supercell`

function was used. The increase in size of the platelet in its x - and y -directions could be adjusted here to choose the size and aspect ratio of the GNP. The plan was also to make the distance between the cell edge and the platelet modifiable, which also modifies the weight percentage of the composite. To do this, only the platelet was isolated from the periodic cell using

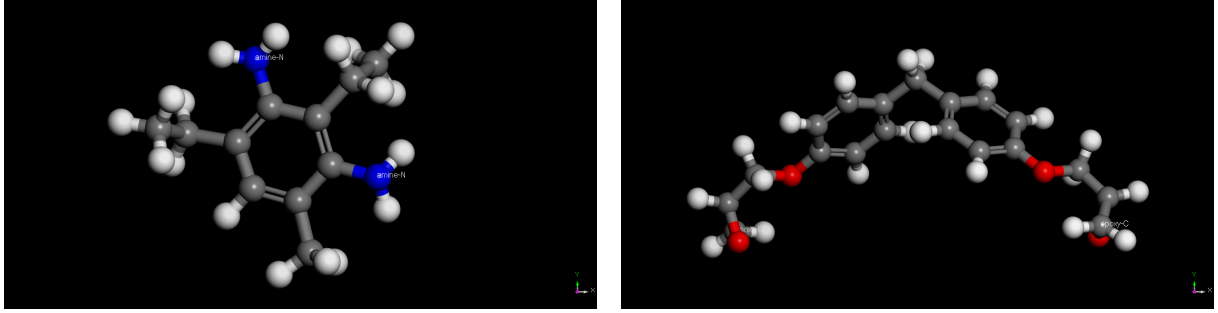
`Build → Symmetry → Nonperiodic Superstructure`

and then it was copied into a new document with a larger cell which could be varied in size. The plate was then moved to the middle of the cell by first reading the coordinates of its atoms and measuring their distance to the cell edge. A function to rotate the plate arbitrarily was also implemented.

3.2 Packing and optimising geometry

Using the

`Amorphous cell → Packing`



(a) The DETDA molecule shown in the Materials Visualizer.

(b) The DGEBF molecule shown in the Materials Visualizer.

Figure 3.1: The components of the epoxy resin system.

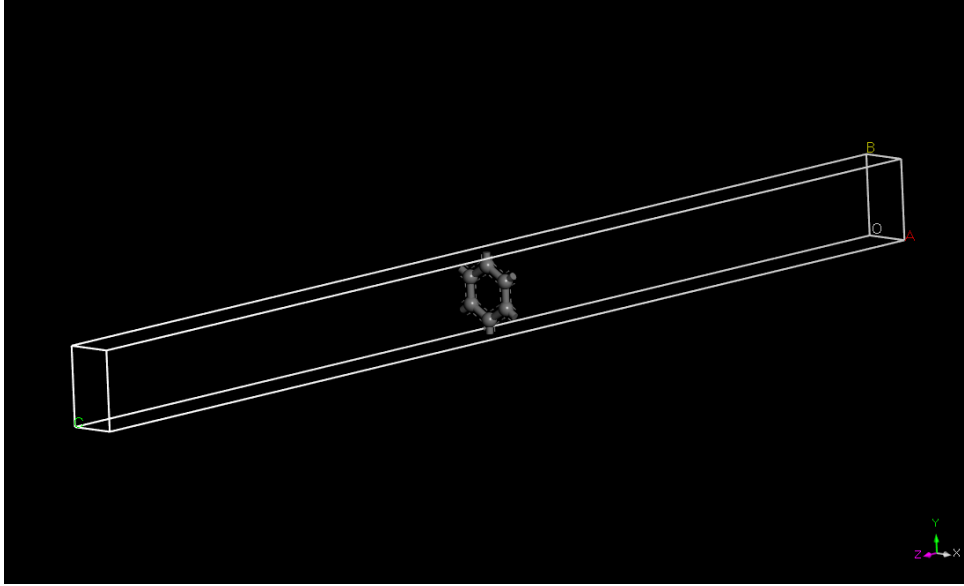


Figure 3.2: A single hexagon of graphene shown in the Materials Visualizer. The white lines around the hexagon mean that it is a periodic cell.

module, the DGEBF and DETDA molecules were packed into the cell around the GNP. This was done with a density of 0.9 g/cm^3 . Using the Forcite Geometry Optimization module, the geometry of the cell was then optimised. This was done in two steps, where the first step was to optimise with the steepest descent method with a maximum of 4000 iterations and the convergence criteria $\Delta E = 10^{-4} \text{ kcal/mol}$, $\Delta F = 3 \cdot 10^{-3} \text{ kcal/mol/\AA}$ and $\Delta u = 5 \cdot 10^{-5}$, where ΔE is the energy difference, ΔF is the force difference and Δu is the displacement difference. The second step was to optimise using the conjugate gradient method with the same convergence criteria and maximum number of iterations = 3000.

3.3 Equilibration and cross-linking

The cross-linking algorithm was inspired by the one in [20, pp. 6838–6839]. Described in pseudo-code, the steps of the algorithm were:

- **INITIATION**

- Build GNP
- Label the reactive carbon atoms on the epoxy rings and the reactive nitrogen atoms on the amine groups
- Pack cell with molecules
- Optimise geometry
- Define cross-linking density limit c_{lim}
- Define bond cut-off distance $d_{\text{cut-off}}$
- Count the number of epoxy groups, i.e. the number of potential bonds

- **WHILE** cross-linking density $c \leq c_{\text{lim}}$

- Find all pairs of reactive atoms with distance $d \leq d_{\text{cut-off}}$
- If one nitrogen atom is close enough to two different carbon atoms (or vice versa), save the pair with the smallest distance.
- Create the best fit plane that the GNP atoms span and save its normal vector
- Iterate through the five closest pairs
 - * **IF** the line between the atoms in the pair does not cross the plane
 - Delete one hydrogen-nitrogen bond on the amine group
 - Delete the carbon-oxygen bond on the epoxy group
 - Create a bond between the nitrogen atom and the carbon atom
 - Create a bond between the hydrogen atom and the oxygen atom
- Update the number of bonds created, i.e. cross-linking density
- Optimise structure geometry
- Equilibrate with NPT and NVT

This cross-linking scheme was implemented in PowerShell, Python and Perl scripts.

3.4 Calculating material parameters

The cross-linked structure went through more geometry optimisation before equilibration to avoid large energy differences between the time steps. The system was equilibrated using NPT for 50 ps, with a Berendsen barostat, a velocity-scaling thermostat and a time step of 1 fs Ewald vdW summation method and Particle-Particle-Particle-Mesh (PPPM) electrostatic summation method. The same summation methods were used in a study of a similar material [21]. The structure was equilibrated further with constant NVT, with the same settings but with Berendsen thermostat instead. Materials Studio had methods to determine the material parameters from the MD simulation data by using the Forcite Mechanical Properties module. It had three options: the Constant strain method, the Static method and the Stress fluctuation method [10]. In addition to these methods, a method using strain fluctuations adapted from [22] was investigated.

3.4.1 Constant strain method

The constant strain method was based on applying small strains to the structure in one of the six directions xx , yy , zz , yz , zx and xy at a time and recording the resulting stress induced by the applied strain. For this calculation, a maximum strain amplitude was given as a parameter as well as a number of steps. For a maximum strain amplitude = 0.3% and number of steps = 4, the values $\{-0.3\%, -0.1\%, 0.1\%, 0.3\%\}$ were used to create

a 3×3 strain matrix

$$[\varepsilon]^{(3 \times 3)} = \frac{1}{2} \begin{bmatrix} 2\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & 2\varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & 2\varepsilon_{zz} \end{bmatrix}. \quad (3.1)$$

The strain matrix $[\varepsilon]^{(3 \times 3)}$ is then used to calculate the so-called metric tensor

$$G_{ij} = h_{ik}^T \left[2[\varepsilon]_{kl}^{(3 \times 3)} + \delta_{kl} \right] h_{lj} \quad (3.2)$$

where h_{ij} is formed from the cell lattice vectors as in equation (2.7). From G_{ij} , new lattice parameters could be derived and the stress matrix was calculated from geometry optimisation of the strained molecular structure. A linear fit of the strain and stress then gave the Hooke tensor.

3.4.2 Static method

The static method calculates the Hooke tensor of the structure from the second derivative of the potential energy with respect to strain. The Hooke tensor is calculated in this method as follows:

$$C_{ijkl} = \frac{1}{V_0} \frac{\partial^2 U}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \bigg|_{\varepsilon=0}. \quad (3.3)$$

This does not require geometry optimisation like the constant strain method does. However, it only applies to temperatures near 0 K [10].

3.4.3 Stress fluctuation

The third built-in method was based on analysing stress fluctuations to calculate the material parameters. For this, an NVT production simulation has to be done first to allow the internal stress to fluctuate. A thermostat that correctly samples the canonical ensemble has to be used, e.g. the Nosé-Hoover thermostat. The internal stress is calculated as

$$\sigma_{ij} = \frac{1}{V} \left(\sum_{\alpha=1}^N m^{(\alpha)} v_i^{(\alpha)} v_j^{(\alpha)} + r_i^{(\alpha)} f_j^{(\alpha)} \right) \quad (3.4)$$

where V is the constant volume, the superscript (α) denotes the atom and $i, j = 1, 2, 3$, $m^{(\alpha)}$ is mass of atom α , $v_i^{(\alpha)}$ is velocity in direction i , $r_i^{(\alpha)}$ is position component i and $f_i^{(\alpha)}$ is the force acting in the i direction [10]. The Hooke tensor also has other contributions to consider in addition to the stress fluctuation contribution. There are three contributions

$$C_{ijkl} = C_{ijkl}^B + C_{ijkl}^k - C_{ijkl}^f \quad (3.5)$$

and

$$C_{ijkl}^B = \frac{1}{V} \left\langle \frac{\partial^2 U}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \right\rangle, \quad (3.6)$$

$$C_{ijkl}^k = \frac{2Nk_B T}{V} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (3.7)$$

$$C_{ijkl}^f = \frac{V}{k_B T} (\langle \sigma_{ij} \sigma_{kl} \rangle - \langle \sigma_{ij} \rangle \langle \sigma_{kl} \rangle). \quad (3.8)$$

C_{ijkl}^B is the Born term and comes from the second derivative of the potential energy w.r.t. strain and can be calculated numerically by applying small strains in each of the six strain directions mentioned in section 3.4.1 and calculating the energy difference at each step. C_{ijkl}^k is the kinetic contribution and comes from momentum contributions. C_{ijkl}^f is the term that is calculated from the fluctuations of the stress. As the temperature approaches 0 K the atoms stop moving which means that $C_{ijkl}^k, C_{ijkl}^f \rightarrow 0$, which only leaves the Born term. This is the approximation that results in the Static method in section 3.4.2.

3.4.4 Strain fluctuation method

Similarly to the stress fluctuation method, the strain fluctuations can be analysed to calculate the material parameters. For calculating the bulk and shear moduli at a specific temperature, the volume fluctuations from an NPT ensemble simulation are used. The Martyna-Tobias-Klein barostat and Nosé-Hoover thermostat were used, since they render physically correct cell parameter fluctuations. The compliance tensor (inverse of the Hooke tensor) in Voigt notation can then be calculated as

$$[S]_{\mu\nu} = \frac{\langle V \rangle}{k_B T} (\langle \varepsilon_\mu \varepsilon_\nu \rangle - \langle \varepsilon_\mu \rangle \langle \varepsilon_\nu \rangle) \quad (3.9)$$

where ε_μ and ε_ν are the components of the strain tensor in Voigt notation and $\mu, \nu = 1, 2, \dots, 6$. The strain tensor component fluctuations are in turn calculated from the fluctuations of the cell vectors. The transformation matrix of the deformation, i.e. the deformation gradient tensor is given by

$$\mathbf{J} = \mathbf{h} \langle \mathbf{h} \rangle^{-1}. \quad (3.10)$$

The Green-Lagrange strain tensor is then

$$\mathbf{E} = \frac{1}{2} (\mathbf{J}^T \mathbf{J} - \delta), \quad (3.11)$$

which for small fluctuations (the linear elasticity assumption) is translated to

$$\varepsilon_1 = E_{11}, \varepsilon_2 = E_{22}, \varepsilon_3 = E_{33}, \varepsilon_4 = 2E_{23}, \varepsilon_5 = 2E_{13}, \varepsilon_6 = 2E_{12}. \quad (3.12)$$

The components of the Hooke tensor are then calculated by inverting the compliance matrix. The strain fluctuation method does not require any finite applied strains or any geometry optimisations; instead a production simulation is performed to get the trajectories of the volume and the cell parameters. This is done by sampling the isobaric-isothermic ensemble, which allows for fluctuations of the cell edges and angles [22]. After investigating the methods, this was the method used for the final results.

4

Results and discussion

4.1 Cross-linking

The cross-linking approach was successful both for simulations with and without a GNP. In Figure 4.1 a cell with 16 DGEBF and 8 DETDA molecules can be seen where 80% cross-linking has been reached and the approach was also successful for systems of more atoms.

4.2 Mechanical properties

The compliance matrix of the material was calculated from two different production runs from the cell parameter trajectories with the method described in section 3.4.4. This was done on an 80% cross-linked structure with a GNP sheet with dimensions 21.651 Å x 17.9 Å surrounded by epoxy consisting of 119 DGEBF and 59 DETDA molecules. The weight percent of the GNP was then 3.37%. The two production runs lasted 50 ps and 100 ps, respectively and the resulting Voigt form compliance matrix components with error estimates (calculated from statistical inefficiency [23]) can be seen in Tables 4.1 and 4.2 respectively. From the assumption that the material is anisotropic, the compliance matrix element values were used to calculate the Young's moduli and Poisson ratios of the material as

$$E_{ii} = \frac{1}{S_{ii}}, \quad (4.1)$$

$$\nu_{ij} = -\frac{S_{ji}}{S_{ii}} \quad (4.2)$$

$i, j = 1, 2, 3$ and their values can be seen in Tables 4.3 and 4.4.

As shown in Tables 4.1 and 4.2 the, values differ substantially depending on how long the production simulation is, which can also be seen in the derived Young's moduli and Poisson ratios. The relative errors of the compliance tensor are also large and sometimes the error is even larger than the value itself. However, the relative errors were somewhat smaller for the longer simulation. It can be concluded that a convergence study of the simulation length could be interesting.

It can also be concluded that the values of the Young's moduli shown in Table 4.3 are of the same order of magnitude as experimental values with similar weight percent in [19, p. 4128] where the tensile modulus was measured to be 3.04 ± 0.03 GPa at a GNP weight fraction of 3% and 3.15 ± 0.04 GPa with GNP weight percent 4%.

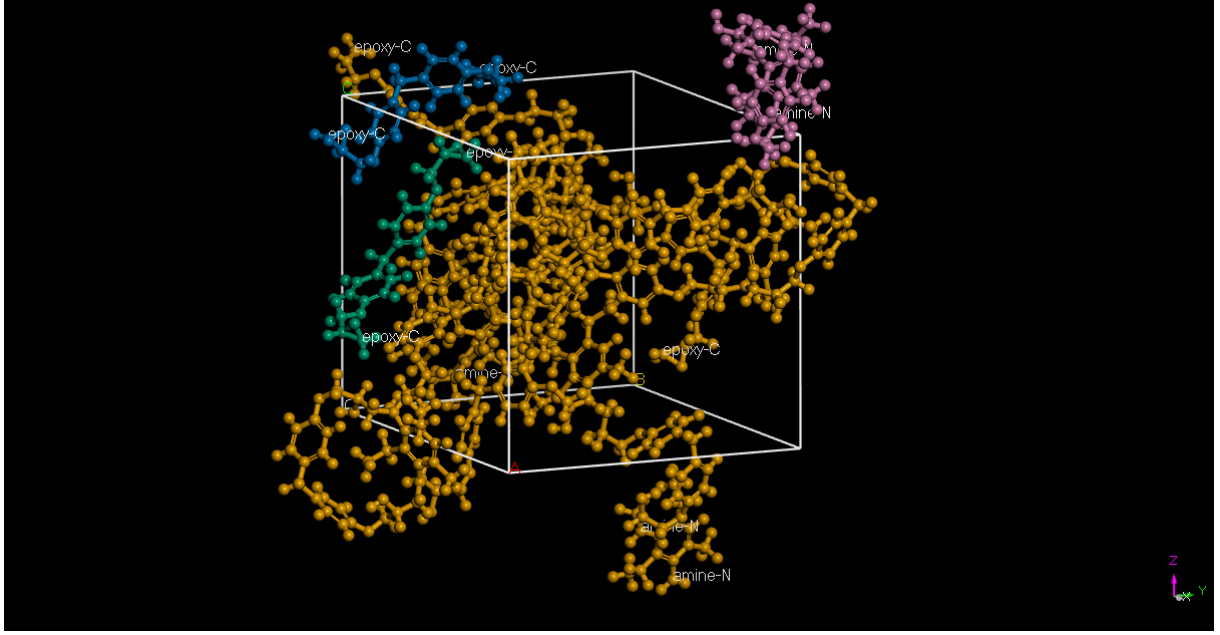


Figure 4.1: A cell without a GNP. The four colours represent the four polymer chains that were created in the simulated curing process.

Table 4.1: The resulting compliance matrix components from the 50 ps simulation with error. The unit is TPa^{-1} .

	1	2	3	4	5	6
1	631 ± 124	-186 ± 82	-335 ± 93	275 ± 154	295 ± 173	-65 ± 136
2	-186 ± 82	392 ± 94	-126 ± 95	-114 ± 128	-209 ± 126	176 ± 96
3	-335 ± 93	-126 ± 95	533 ± 93	-107 ± 130	-8 ± 137	-88 ± 109
4	275 ± 154	-114 ± 128	-107 ± 130	1924 ± 527	339 ± 247	-259 ± 317
5	295 ± 173	-209 ± 126	-8 ± 137	339 ± 247	1935 ± 414	-259 ± 267
6	-65 ± 136	176 ± 96	-88 ± 109	-259 ± 317	-259 ± 267	1253 ± 231

Table 4.2: The resulting compliance matrix components from the 100 ps simulation with error estimates. The unit is TPa^{-1} .

	1	2	3	4	5	6
1	491 ± 77	-201 ± 120	-213 ± 102	193 ± 79	181 ± 99	-8 ± 89
2	-201 ± 120	638 ± 84	-315 ± 60	-227 ± 183	-36 ± 124	229 ± 104
3	-213 ± 102	-315 ± 60	608 ± 88	-21 ± 107	-22 ± 114	-189 ± 94
4	193 ± 79	-227 ± 183	-21 ± 107	1851 ± 412	26 ± 206	-317 ± 194
5	181 ± 99	-36 ± 124	-22 ± 114	26 ± 206	1819 ± 280	-99 ± 178
6	-8 ± 89	229 ± 104	-189 ± 94	-317 ± 194	-99 ± 178	1156 ± 166

Table 4.3: Young's moduli in each of the normal directions, for each of the two production simulations.

	E_{11} [GPa]	E_{22} [GPa]	E_{33} [GPa]
50 ps	1.5860	2.5520	1.8756
100 ps	2.0348	1.5685	1.6450

Table 4.4: *The Poisson ratios, for each of the two production simulations.*

	ν_{12}	ν_{13}	ν_{21}	ν_{23}	ν_{31}	ν_{32}
50 ps	0.2943	0.5309	0.4735	0.3211	0.6278	0.2360
100 ps	0.4086	0.4337	0.3150	0.4937	0.3506	0.5178

5

Ideas for further work

5.1 Simulation work flow

The simulations were done on a personal computer with 24 cores, but Materials Studio provides limited insight into how its computations are parallelised. This meant that all simulations throughout the project were very time-consuming. Investigating if other software, e.g LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) or GROMACS (GROningen MACHine for Chemical Simulations), could be used instead would be a good idea, since they offer greater potential for parallelisation and, more importantly, can be run on Chalmers' computer clusters. One disadvantage of using LAMMPS or GROMACS is that the COMPASS force field cannot be used directly, because it is only available in Materials Studio. It would be necessary to investigate whether other force fields can provide accurate predictions of mechanical properties. One candidate is PCFF, which, like COMPASS, is also a consistent force field. Its accuracy was similar to that of COMPASS in a study of mechanical properties of an epoxy polymer [24], which is promising.

5.2 Creating a surrogate ML model

Since the calculations are computationally expensive, training a surrogate ML model to predict material parameters would be relevant. The training data could be structured so that the aspect ratio, number of GNP layers and weight percent serve as input variables. Then the output data could be the material parameters established through the simulations and with an orientation averaging method, as described in [25] and [26] to get homogeneous properties for a composite with many GNPs with randomly distributed orientations. For only predicting elastic parameters a regular feed-forward neural network can be used and the training data can consist of strain or stress fluctuation method results to calculate the Hooke tensor. An example of this is found in [27].

To model plastic material behaviour, however, a regular feed-forward neural network would not be sufficient since it does not account for history. The training data for analysing plasticity would have to be a strain path where the strain and stress are saved as a time series, and that is not suitable for a FFNN. A recurrent neural network (with gated recurrent units) or a transformer would be better suited for training. The pros and cons of those two architectures are discussed in [28] and [29].

6

Conclusion

The elastic properties of a GNP/epoxy composite were investigated using molecular dynamics simulations and the strain fluctuation method. A computational workflow was developed for constructing and cross-linking the polymer of the composite and calculating its compliance tensor. The calculated Young's moduli were of the same order of magnitude as experimental values, but the results showed substantial statistical uncertainty and variation between simulation times. Therefore, the present simulations do not provide sufficient convergence for reliable quantitative prediction. Nevertheless, the main findings were:

- The establishment of a workflow for constructing, cross-linking and performing MD simulations of the GNP/epoxy composite.
- The calculation of the elastic properties, which were found to be of the same order of magnitude as experimental results, but with variation between the 50 ps and 100 ps simulations.
- The identification of simulation duration and statistical convergence as the main limitations, demonstrating the need for longer simulations and convergence studies.

Future work should focus on longer simulations using high-performance computing to establish convergence. The workflow could then be extended to investigate different composite parameters and generate data for surrogate machine-learning models.

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