

Molecular Dynamics Calculations for Multiscale Materials Modeling

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0.1 Introduction

This report details the simulation of various molecular scale events. The Molecular Dynamics (MD) method is used to simulate inter-particle interactions.

0.2 Background

Molecular Dynamics methods treat the interactions of individual atoms in a lattice to determine the behavior of a material on the atomic scale. Atoms are arranged on a lattice representing the initial structure of the model. The positions of the atoms are updated according to forces that result from the potentials chosen for the problem at hand. By studying the changing structure of the atoms, a material's response to external forces can be understood.

0.3 Methods

0.3.1 Copper Nanowire



Figure 1: The stress Initial Condition.

Of interest is the simulation of a copper Nanowire's response to deformation. Simulations were carried out using Nanohub's Nanowire Tensile Deformation Lab (NTDL) module. A lattice of atoms was generated of size

20 x 20 x 130 Å. As per the assignment's direction, the NTDL parameters were set to 8 x 8 x 36 to produce this initial condition. The structure was set to be a free surface in each direction, with a tensile force applied to each end 0.3.1. The tensile stress was implemented by applying a displacement of 0.02 Å every 20 simulation time steps. 30,000 time steps were performed. The simulation was carried out a second time, with the cross sectional area doubled (40 x 40 x 130 Å).

0.3.2 Collagen Stretching



Figure 2: The stress initial condition.

To be investigated is the behavior of a collagen analog when subjected to a tensile force. The software used the package Stretching Simulation of an Alpha-Helical Protein Domain (SSAPD). SSAPD uses the method of Steered Molecular Dynamics (SMD) with a CHARMM force field to simulate the interaction of the molecule's components. The boundary conditions are those indicated in 0.3.2. Molecule data, including initial positions of atoms, points of fixation, and force field potentials were provided. The SSAPD module was given the parameters according to:

DCD Freq.	Velocity	Steps	Averaging Bins
150	0.0005	150,000	300

0.4 Results

0.4.1 Copper Nanowire

The raw results of the stress tensor are given in 0.4.1 and 0.4.1 for each cross section tested. The value of interest is the Young's modulus in the direction of displacement. To obtain this value, the data is taken for ϵ_{zz} vs σ_{zz} over the linear elastic range. The linear elastic range was visually determined to be the first 5250 and 6750 time steps for the small and large cross sections, respectively. The Young's Modulus is the slope of the elastic range. Time step (x) is converted to strain, and simulation stress is modified according to $1 \text{ (eV/\AA}^3) = 160 \text{ GPa}$. 0.4.1 and 0.4.1 show the fit and Young's Modulus

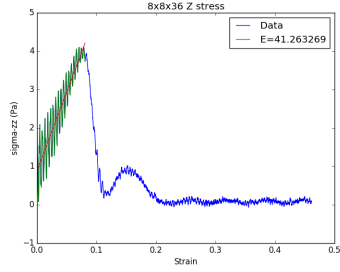


Figure 3: Fit for 8x8x46 nanowire.

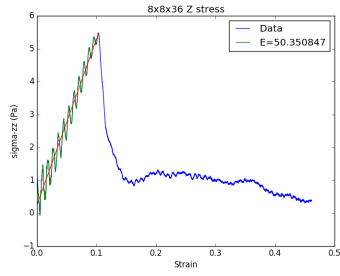


Figure 4: Fit for 16x16x46 nanowire.

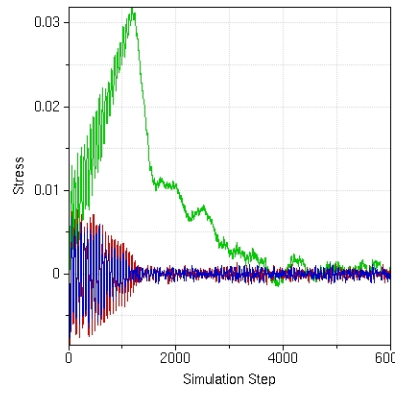


Figure 5: Stress tensor for 8x8x16 nanowire. Step size is sim-step*5.

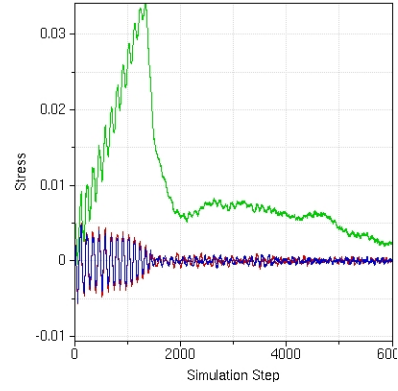


Figure 6: Stress tensor for 16x16x36 nanowire. Step size is sim-step*5.

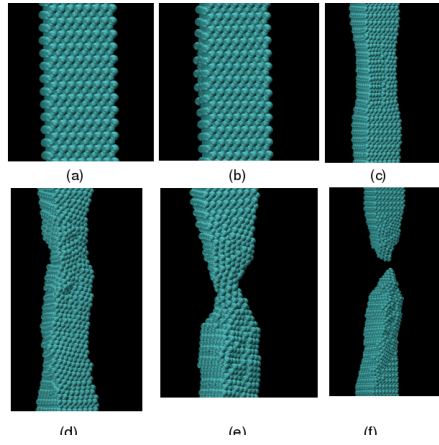


Figure 7: Stretching evolution of 8x8x36 nanowire.

to be 41 and 50 GPa, respectively. We find that the Young's modulus is not strongly sensitive to changes in wire aspect ratio, as a doubling of the aspect ratio results in a 20 percent increase in E . It is of interest to compare this value to that of a macroscopic sample, where $E_{bulk} = 117$ GPa. According to [2], the MD calculated Young's Modulus can be compared to the bulk value by considering the thickness of the nanowire. For the small case, the correction factor of around 0.7 results in a true $E = 58.9$ GPa, leaving a significant discrepancy.

0.4.1 shows the behavior of the wire up until fracture. The wire initially carries the strain induced stress without any dislocations in (a). In (b), the very first visible dislocations occurs near the center of the wire. (c) begins to show narrowing of the central section of the wire, with buldges propogating towards the ends. By (d), significant disorder has arisen and out of plane bending is apparent. (e) exhibits progressive necking to the point of eventual failure, with (f) showing the fracture state and subsequent reduction of stress. The linear elastic region persists until some point between (c) and (d), when the total bonded cross-sectional area begins to decrease and necking commences. σ_z decreases as necking proceeds until reaching approximately zero at fracture.

0.4.2 Collagen Stretching

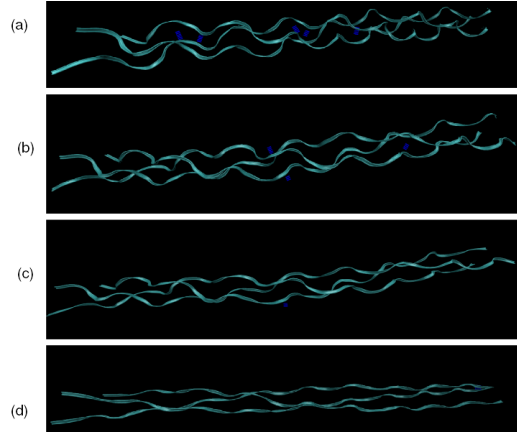


Figure 8: Stretching of collagen molecule.

Using VMD, the initial length of the molecule was estimated to be 81 Å. The output log provided information regarding the computation rate, and reported requiring 0.0464128 CPUsec/sim step and 0.537186 CPUdays/ns.

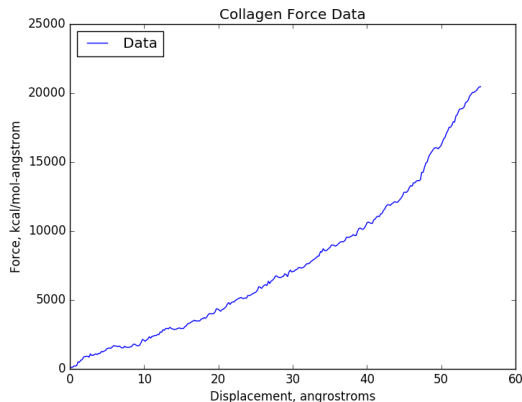


Figure 9: Force data for collagen stretching.

This converts to roughly 1 fs per simulation time step, or 150 ps of total simulation time. The velocity used was $0.005 \text{ \AA} / \text{time step}$ (50 m/s). This at first glance seems high, but considering the velocity of a thermal free neutron at room temperature (2200 m/s), is likely within an order of magnitude of the vibrational "velocity" of collagen.

From 0.4.2, we can observe the stretching behavior of collagen. (a) shows the molecule in its relaxed state, with a handful of hydrogen bonds present. (b) shows the molecule's initial response to strain, with a slight reduction in hydrogen bond count and the initial unraveling of the strands. In (c), few hydrogen bonds remain. (d) shows the molecule almost completely unravelled, but before any major fracture has occurred. It is expected that simulation of further stretching would cause strand failure.

From 0.4.2, it is found that the Youngs modulus is 1100 GPa. This does not agree with the value of 2 GPa for displacements larger than 10 percent [5].

Bibliography

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