Mechanical testing Of Epoxy

Update 04/18

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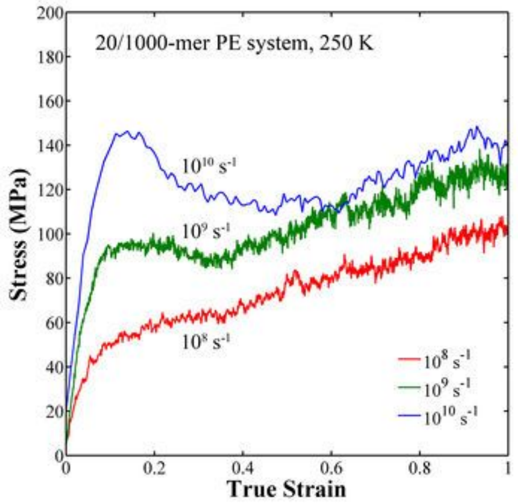
Current objectives:

- Last objective accomplished;
    - Cross linked structure generation for a small system (2 IPD + 2 DGEBA)
- Current objectives:
    - Scale up the system :
        - 216 reactive IPD + 204 reactive DGEBA in 64*64*64 A^3 box
        - It has ~16800 atoms
    - Perform mechanical testing before cross linking (done till here)
    - Do the crosslinking (Stuck here)
        - Wrote a python script to edit the lammps data file at specific locations to mark reactive atoms separately
        - #In the earlier small system I had manually marked them
        - In the scaled up system, while crosslinking, I am getting errors after around 10 crosslinks, trying to fix that
    - Perform mechanical testing after crosslinking and compare differences

An example: Uniaxial testing of polyethylene

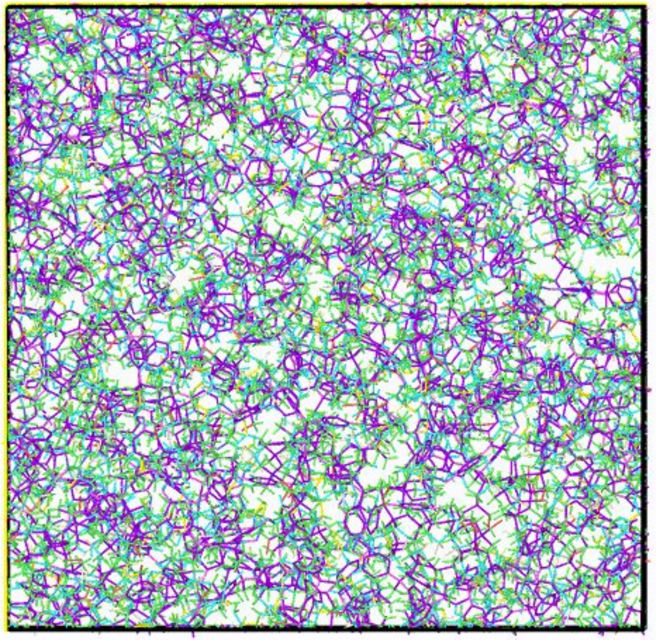
- This shows the results of the MD simulation that attempted uniaxial deformation in 1000 mer polyethylene
- Trends similar to experiments observed at strain rate of $10^{10}s^{-1}$:
  - An elastic regime followed by a yield peak and subsequent softening and strain hardening regimes
  - The smooth curves we see here is regression fit of very noisy data



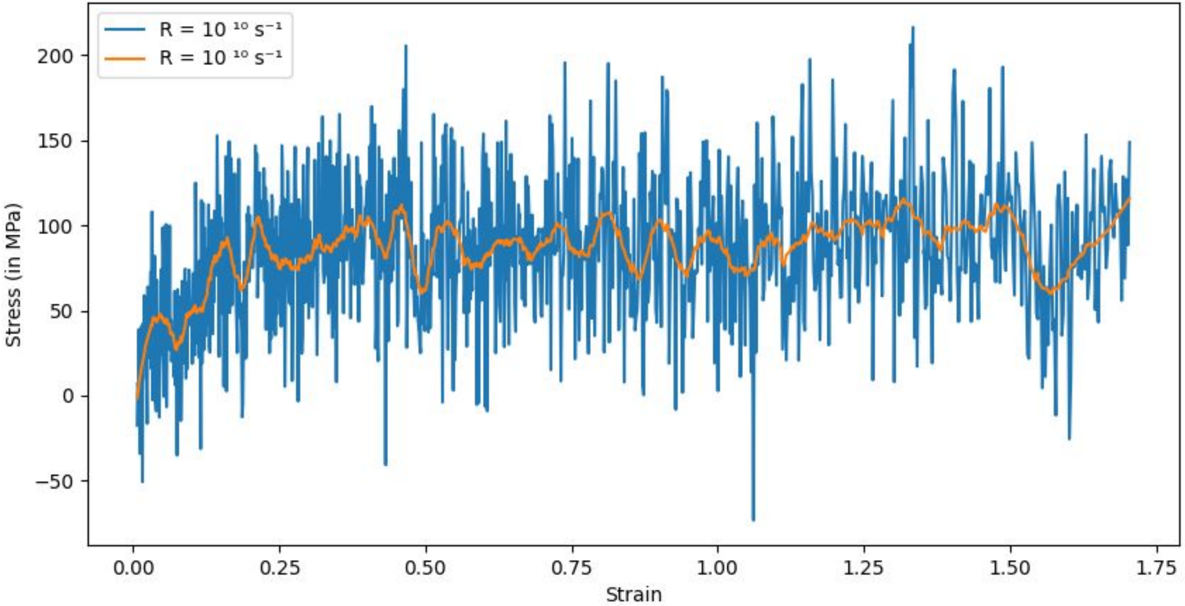
Hossain, D., Tschopp, M.A., Ward, D.K., Bouvard, J.L., Wang, P., Horstemeyer, M.F., "Molecular dynamics simulations of deformation mechanisms of amorphous polyethylene," Polymer, 51 (2010) 6071-6083.

Uniaxial deformation of uncrosslinked epoxy:

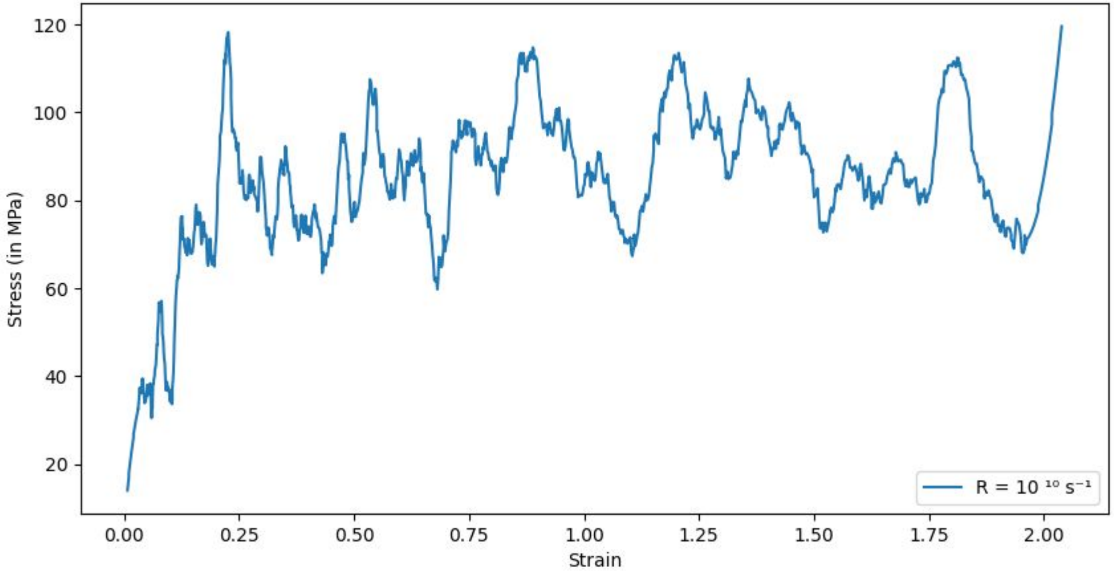
- 216 IPD + 204 DGEBA in a cubic box(64*64*64 $Å^3$), resulting in density of 0.83 g/cm^3
- Uniaxial deformation was done along x, y and z axis
- Strain rate was kept the same as previous example of polyethylene at $10^{10}s^{-1}$.



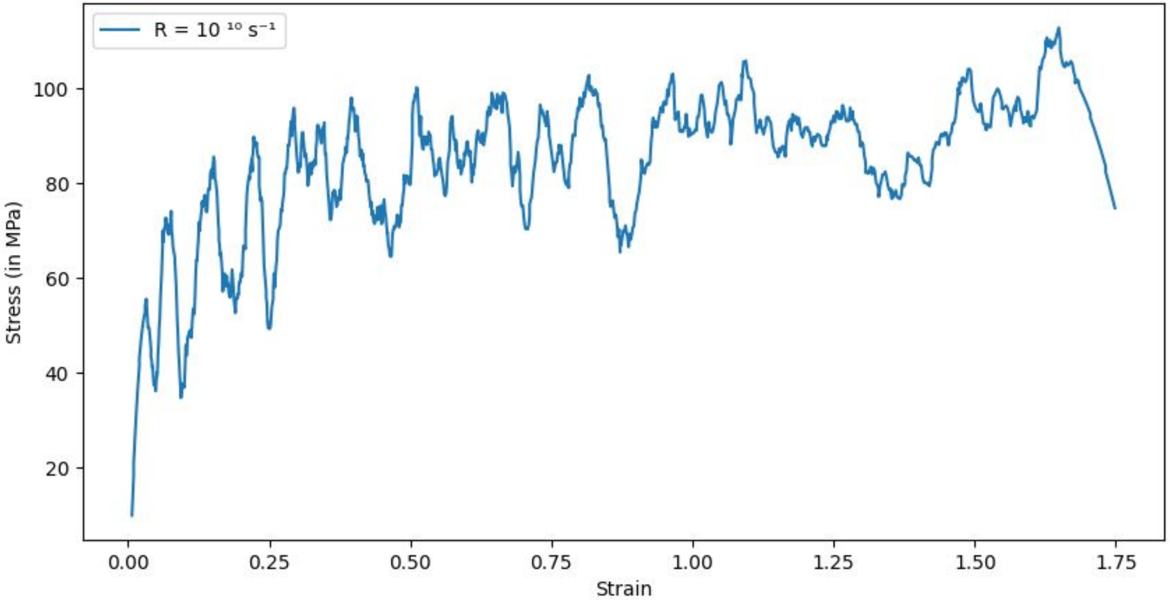
Uniaxial loading -> Fluctuations -> Smoothening



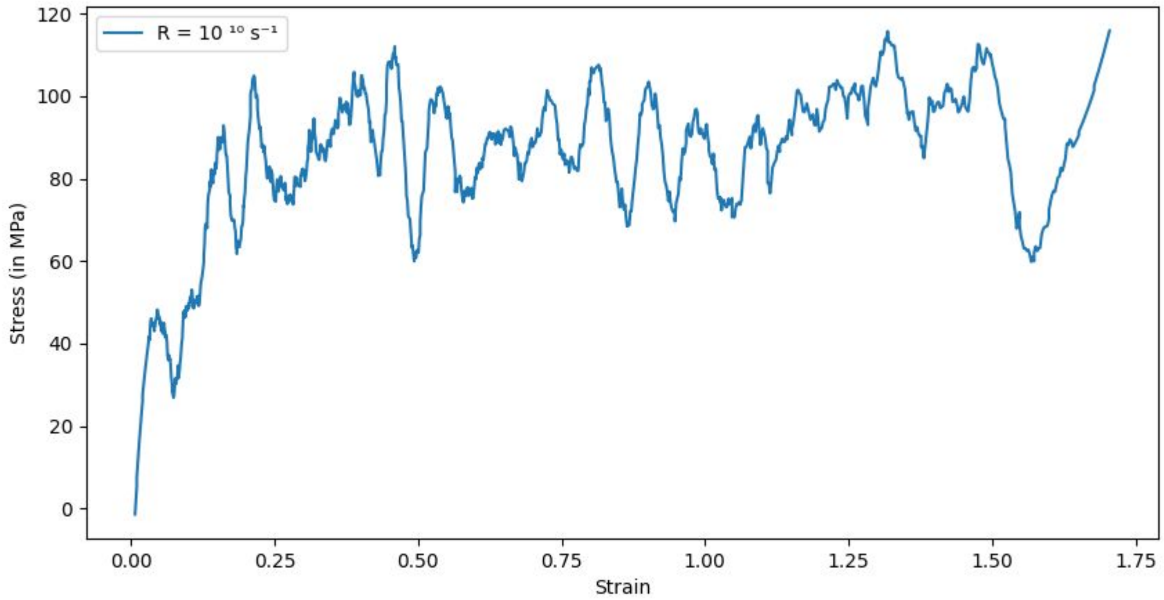
Uniaxial loading along x :



Uniaxial loading along z:

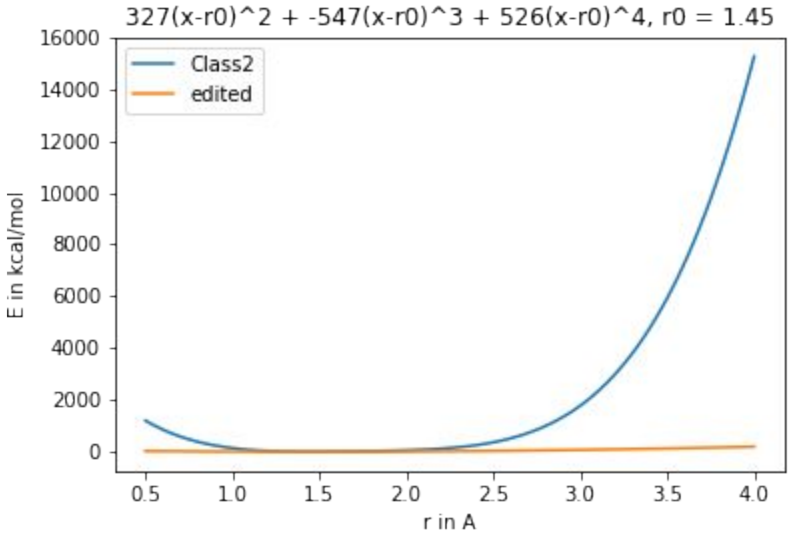


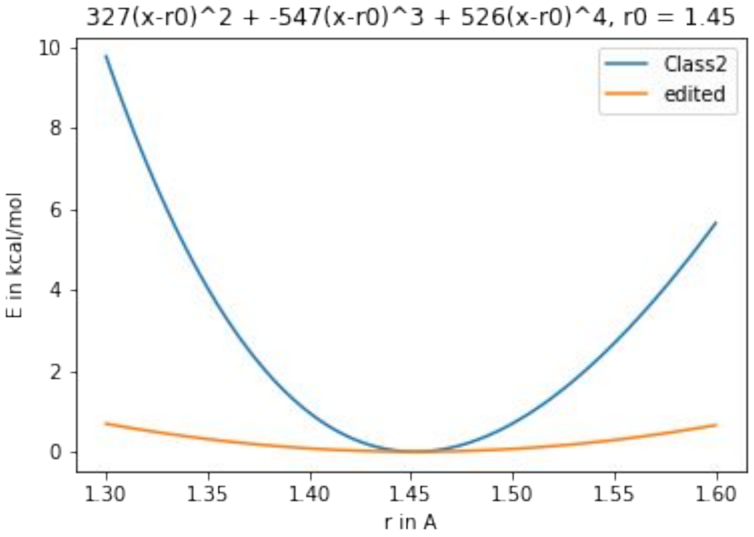
Uniaxial loading along y:



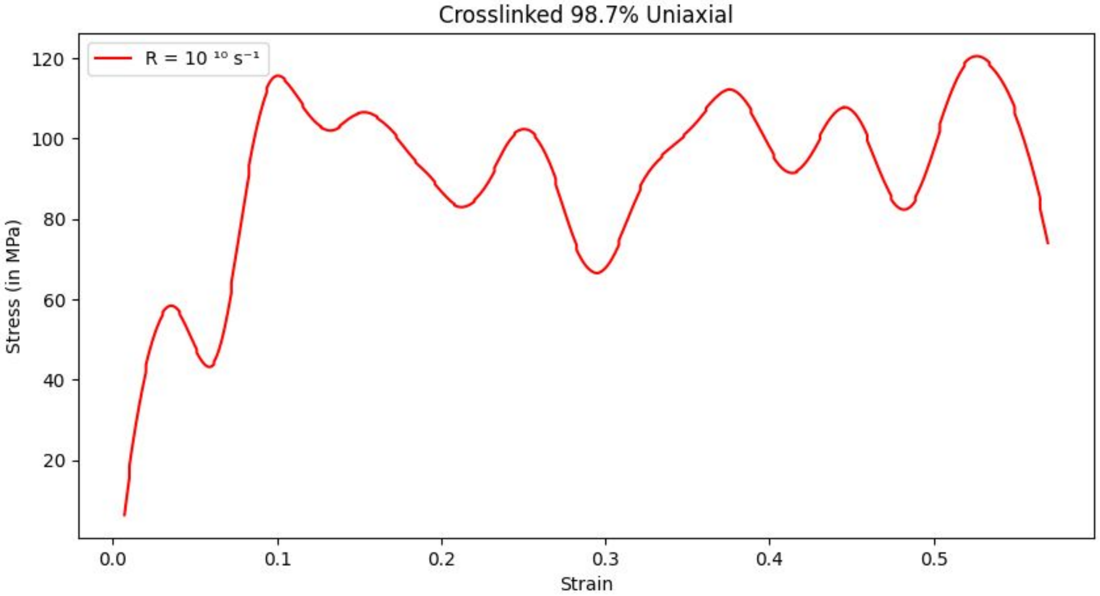
Crosslinked Epoxy

Fixed Error by progressive bond parameter updation.



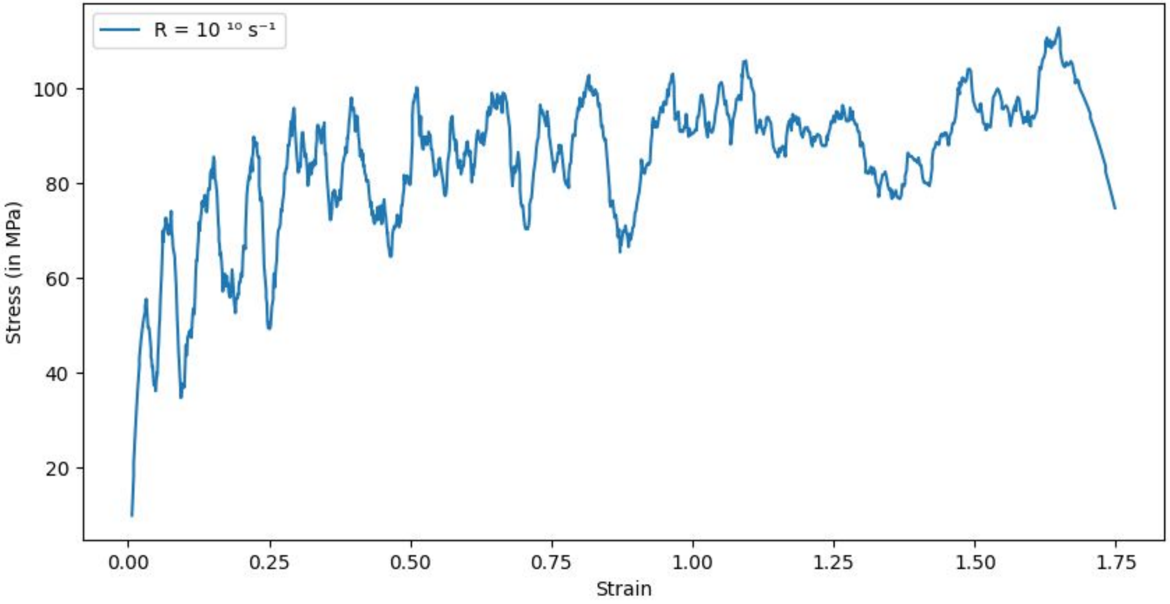


Till 0.5

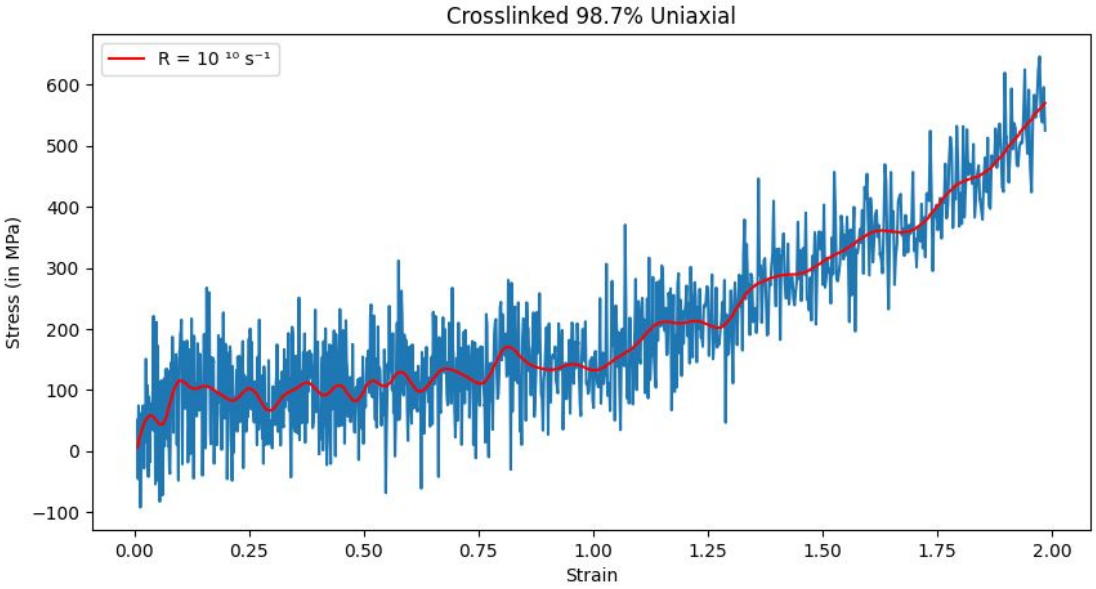


Crosslinked 98.7% Uniaxial
R = 10 ¹⁰ s⁻¹
120
100
80
60
40
20
Stress (in MPa)
0.0
0.1
0.2
0.3
0.4
0.5
Strain

Uniaxial loading of uncrosslinked epoxy:



Uniaxial loading of crosslinked epoxy

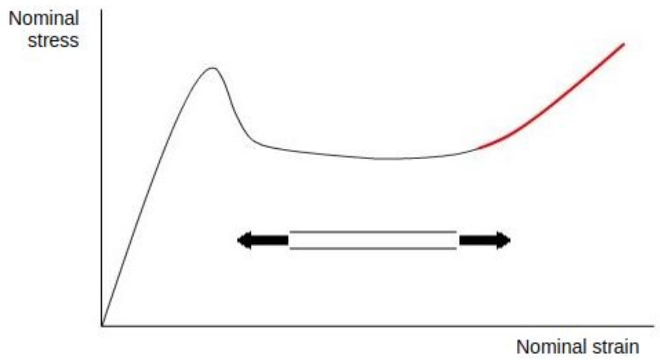


Polymer Stress Strain Curve

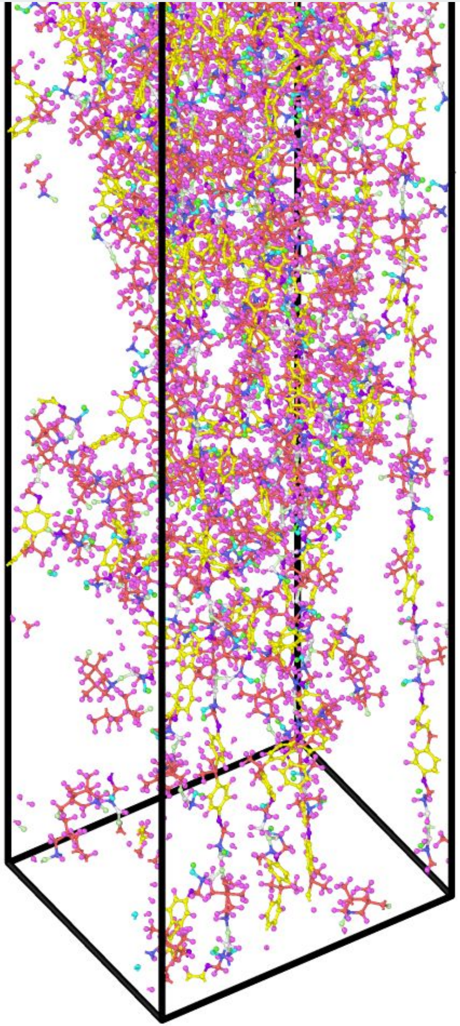
Polymer stress-strain curve

Previous

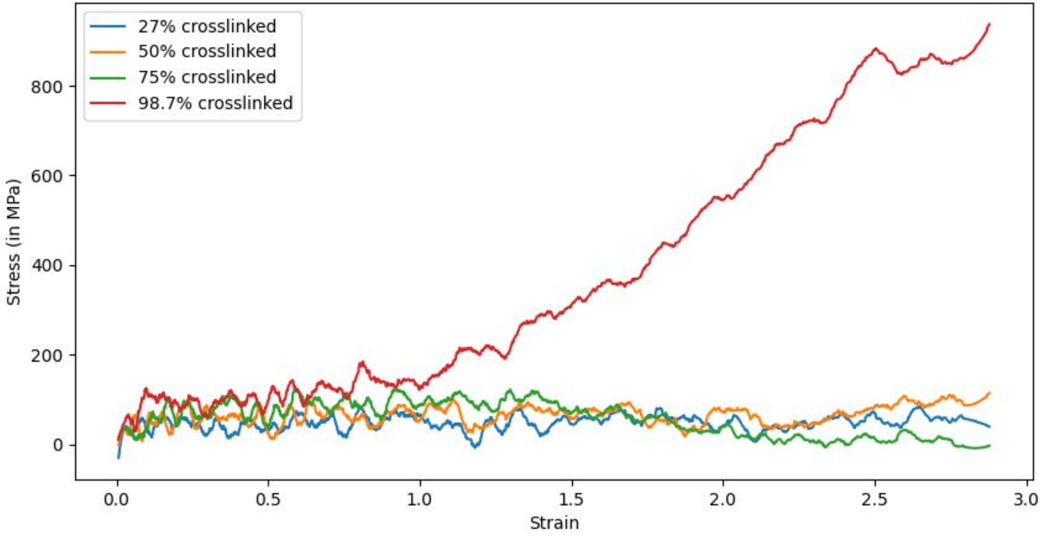
Next

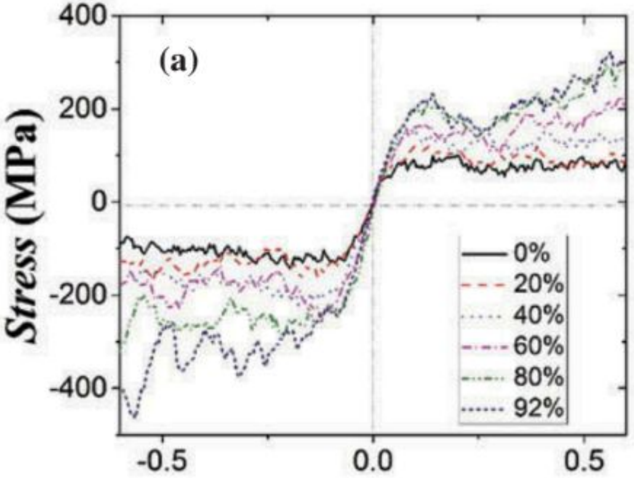


Strain Hardening. The increase in the final section of the curve is a result of strain hardening, which occurs once the whole sample is necked. The stress rises until fracture takes place. Strain hardening is principally a consequence of chain orientation. Molecules are aligned parallel to the stretching direction in the cold drawn regions of both amorphous and crystalline polymers. As a result of the directional nature of covalent bonding, an oriented polymer is significantly stronger and stiffer than an isotropic one. Thus the material in the neck is capable of supporting a much higher stress than that outside the neck. Therefore if they do not first suffer brittle fracture, polymers tend to form stable necks and undergo cold drawing.

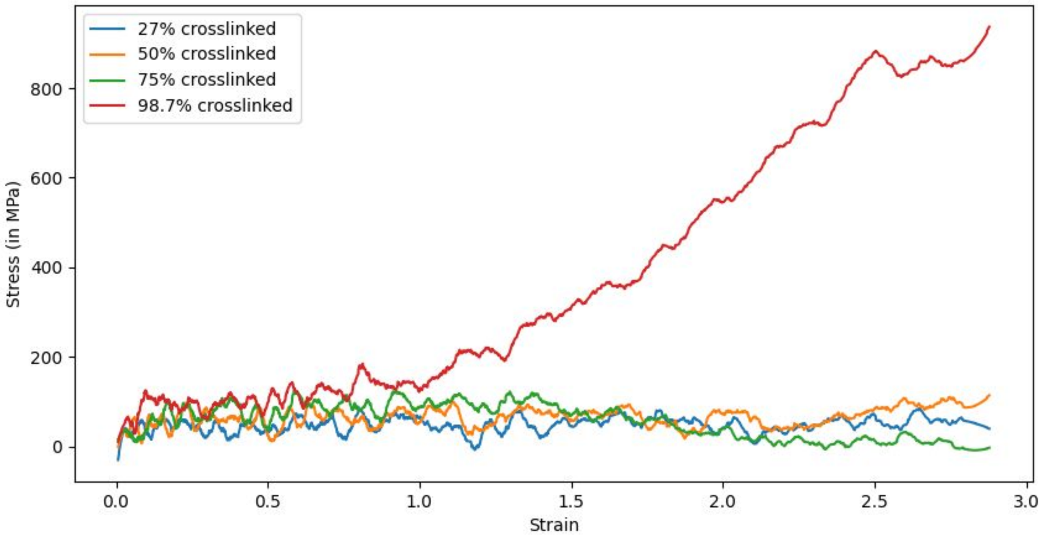


Comparison of loading curves for various degree of crosslinking

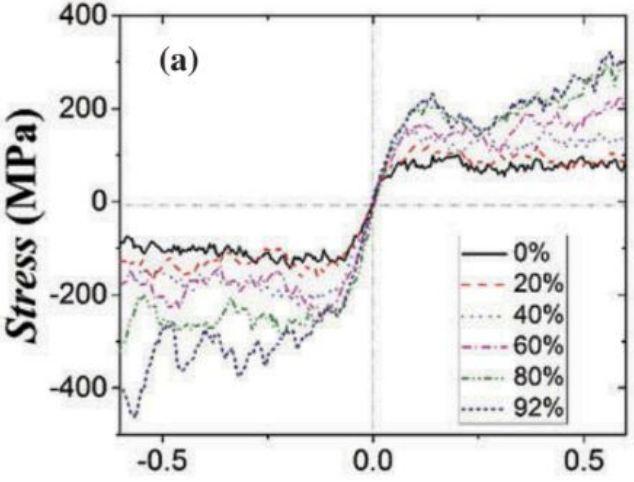




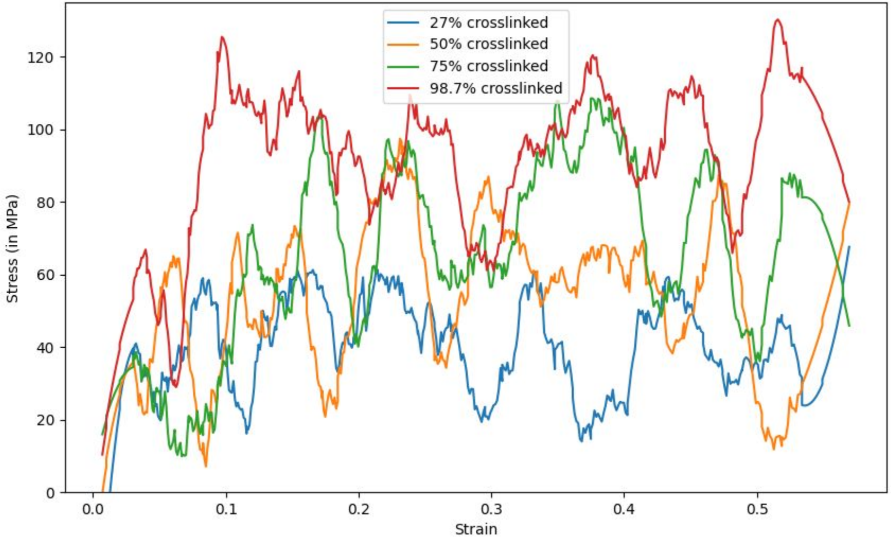
(a)
Stress (MPa)
400
200
0
-200
-400
-0.5
0.0
0.5
0%
20%
40%
60%
80%
92%



27% crosslinked
50% crosslinked
75% crosslinked
98.7% crosslinked
Stress (in MPa)
800
600
400
200
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Strain



(a)
Stress (MPa)
400
200
0
-200
-400
-0.5
0.0
0.5
0%
20%
40%
60%
80%
92%



27% crosslinked
50% crosslinked
75% crosslinked
98.7% crosslinked
Stress (in MPa)
0
20
40
60
80
100
120
0.0
0.1
0.2
0.3
0.4
0.5
Strain

Notes:

- Noise reduction of the data was done by applying Savitzky-golay filter, as otherwise it was too noisy to deduce anything.