

Carbon Nanotube Fracture

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Due to their mechanical properties, carbon nanotubes (CNTs) hold promise as nanoreinforcements in a variety of composites. As a result, numerous theoretical and experimental studies have been performed in order to understand their behavior under axial tension. Whereas quantum mechanical studies typically find failure strains in the range of 20-30% and failure stresses in excess of 100 GPa, the experimental measurements have reported much lower values. Now, researchers believe that this discrepancy occurs because of defects in the nanotubes used in experiments. In this assignment, we will calculate the failure stress and strain for a pristine (non-defected) carbon nanotube.

1. A file containing initial coordinates for a carbon nanotube with 90 carbon atoms (capped by 20 hydrogen atoms) is copied at the bottom of this document (labeled P0). Optimize the equilibrium structure using PM3. You will need to use the IFREEZ option (see the end of this document for more details). Calculate the length and diameter of the nanotube and record its energy.
2. Initial coordinates with incrementally increased x-coordinates are available at the end of this document (files P1-P7). Repeat the previous step with these stretched coordinates. Record the energy, length, and diameter of each nanotube. If the nanotube does not appear on your QC-Lab screen, check to see if the geometry was located successfully. If it was not, consider this to be the point of fracture. Run one more geometry optimization using initial coordinates for the next strain increment and report what happens to the structure. Determine the failure strain for the nanotube.

3. The natural strain (ϵ) of a wire is defined by

$$\epsilon = \frac{L}{L_0}$$

Plot the energy vs. ϵ curve and fit the values to a second-degree polynomial.

4. As a measure of strain, use the stretch, which is defined by

$$\sigma = \frac{L - L_0}{L_0} \equiv \frac{\Delta L}{L_0}$$

where L and L_0 are the current and initial (unstrained) lengths and ΔL is the elongation of the tube. What is the failure strain for this system?

5. The fundamental frequency of vibration of a wire of length L and mass m and tension T is given by

$$f_1 = \frac{1}{2L} \sqrt{\frac{T}{\rho}} = \frac{1}{2L} \sqrt{\frac{T}{m/L}}$$

Assuming similar behavior, with what frequency will a SWCNT(5,5) vibrate if under a tension of 145 GPa its length is 10 mm.

6. A recent measurement that relates to this work is described in: , Bei Peng, Mark Locascio, Peter Zapol, Shuyou Li, Steven L. Mielke, George C. Schatz and Horacio D. Espinosa, Nature Nanotech, 3, 626-631 (2008). How well do the calculated results compare with the results in this paper?

Geometry restraints for the Z-coordinate of the terminal C atoms of the nanotube. Use for Stretch points 1-7.

```
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          96,99,102,105,108,111,114,117,120
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\$END

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H	1.0	0.0683217552	-3.8296681158	-4.5866374463
H	1.0	3.6633434003	-1.1184546801	-4.5866374463
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C	6.0	-3.2776941902	-0.7186332506	-1.3190199796
C	6.0	-0.3294023713	-3.3393423052	-1.3190199796
C	6.0	3.0741123288	-1.3451937940	-1.3190199796
C	6.0	2.2293082757	2.5079668190	-1.3190199796
C	6.0	-1.6963240430	2.8952025309	-1.3190199796
C	6.0	-3.2776941902	0.7186332506	-1.3190199796
C	6.0	-1.6963240430	-2.8952025309	-1.3190199796
C	6.0	2.2293082757	-2.5079668190	-1.3190199796
C	6.0	3.0741123288	1.3451937940	-1.3190199796
C	6.0	-0.3294023713	3.3393423052	-1.3190199796
C	6.0	-3.2776941902	0.7186332506	1.3190199796
C	6.0	-1.6963240430	-2.8952025309	1.3190199796
C	6.0	2.2293082757	-2.5079668190	1.3190199796
C	6.0	3.0741123288	1.3451937940	1.3190199796
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C	6.0	3.2594507174	-0.6977153717	0.0000000000
C	6.0	1.6707924147	2.8843159373	0.0000000000
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P3

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H	1.0	-2.3258578941	2.8213117305	4.9192110629
H	1.0	-3.4019565216	-1.3401890350	-4.9192110629
H	1.0	0.2233331355	-3.6495941055	-4.9192110629

H	1.0	3.5399839902	-0.9153841673	-4.9192110629
H	1.0	1.9644972900	3.0838555773	-4.9192110629
H	1.0	-2.3258578941	2.8213117305	-4.9192110629
H	1.0	-3.4019565216	1.3401890350	-4.9192110629
H	1.0	-2.3258578941	-2.8213117305	-4.9192110629
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C	6.0	-1.6451205641	2.8956627397	4.0676627300
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C	6.0	3.1877165203	-0.6849075748	2.6747314908
C	6.0	1.6364443901	2.8200504886	2.6747314908
C	6.0	-2.1763382665	2.4277946267	2.6747314908
C	6.0	-2.9814954098	-1.3195908916	-2.6747314908
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C	6.0	3.0310895740	-1.3348692884	1.3121331380
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C	6.0	-1.6675864953	2.8615616896	1.3121331380
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C	6.0	1.6928177477	2.8848046778	0.0000000000
C	6.0	-2.2205028346	2.5014190207	0.0000000000
C	6.0	-3.0651639716	1.3388427029	0.0000000000
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P4

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H	1.0	0.2653576777	-3.6587356419	-5.1638851964
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H	1.0	1.9358719815	3.1159526418	-5.1638851964
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C	6.0	2.2205319420	2.4342193438	4.3676627300
C	6.0	-1.6288980624	2.8640665183	4.3676627300
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P5

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C	6.0	-3.1536408148	-0.6736211501	-1.4863816355
C	6.0	-0.3338768216	-3.2074510301	-1.4863816355
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C	6.0	-2.1619928813	2.4037232675	0.0000000000
C	6.0	-2.9541692189	1.3133860785	0.0000000000
C	6.0	-2.1619928813	-2.4037232675	0.0000000000
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C	6.0	3.1619620699	0.6738654420	0.0000000000
C	6.0	0.3362158955	3.2154405043	0.0000000000
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P6

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H	1.0	-2.4238831556	2.8223173344	5.4699970356
H	1.0	-3.4332043794	-1.4331058500	-5.4699970356
H	1.0	0.3020461588	-3.7080254592	-5.4699970356
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C	6.0	-1.6274341257	2.8837807161	4.7426627300
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C	6.0	3.0116656407	1.3764458292	-4.7426627300
C	6.0	-0.3784219109	3.2896093856	-4.7426627300
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P7

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