

Electronic Supplementary Information

Mechanical characteristics and failure behavior of puckered and buckled allotropes of antimonene nanotubes: A molecular dynamics study

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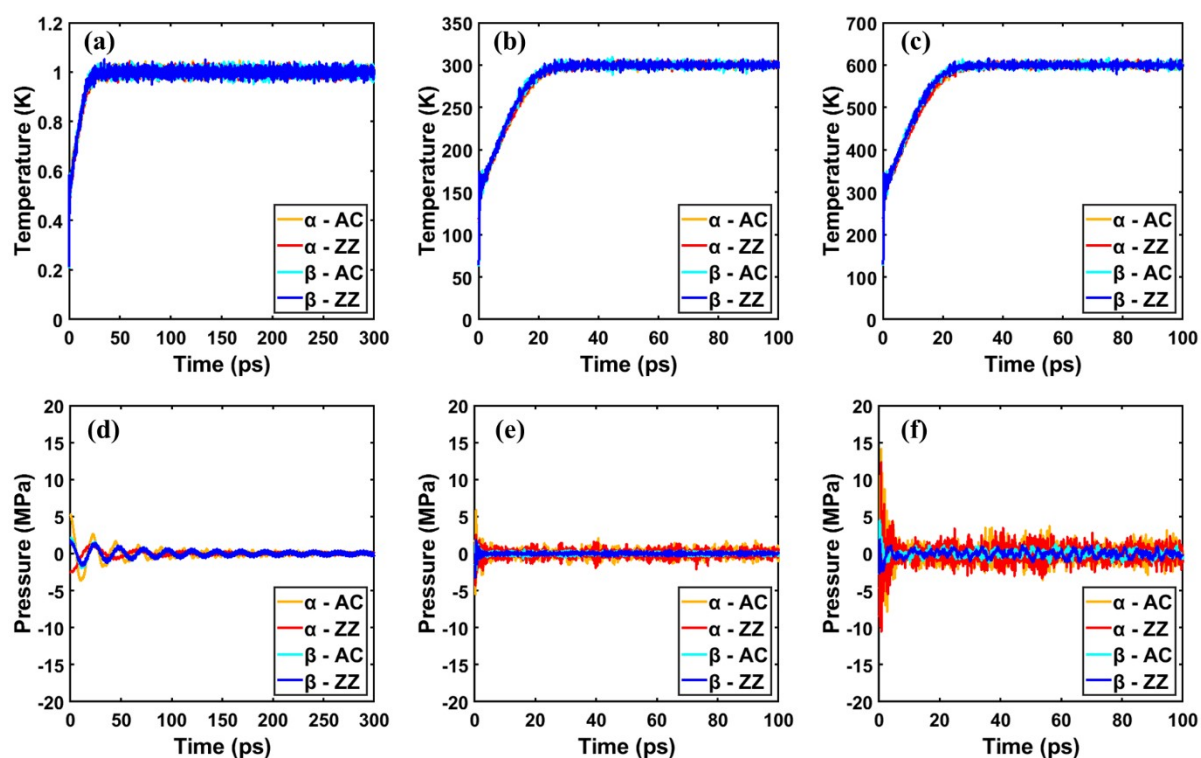


Figure S1. Temperature (a-c) and pressure (d-f) profiles of the antimonene nanotube specimens within the equilibration period at 1, 300, 600 K, respectively.

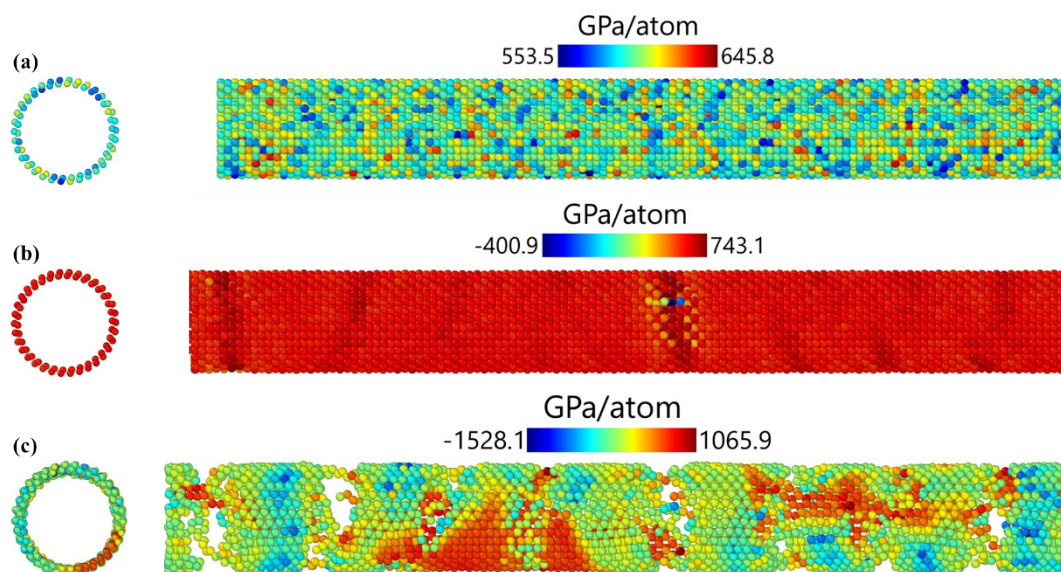


Figure S2. Axial stress distribution of armchair β -SbNT specimen for the strain states of (a) 33%, (b) 34%, and (c) 35% at 1 K temperature.

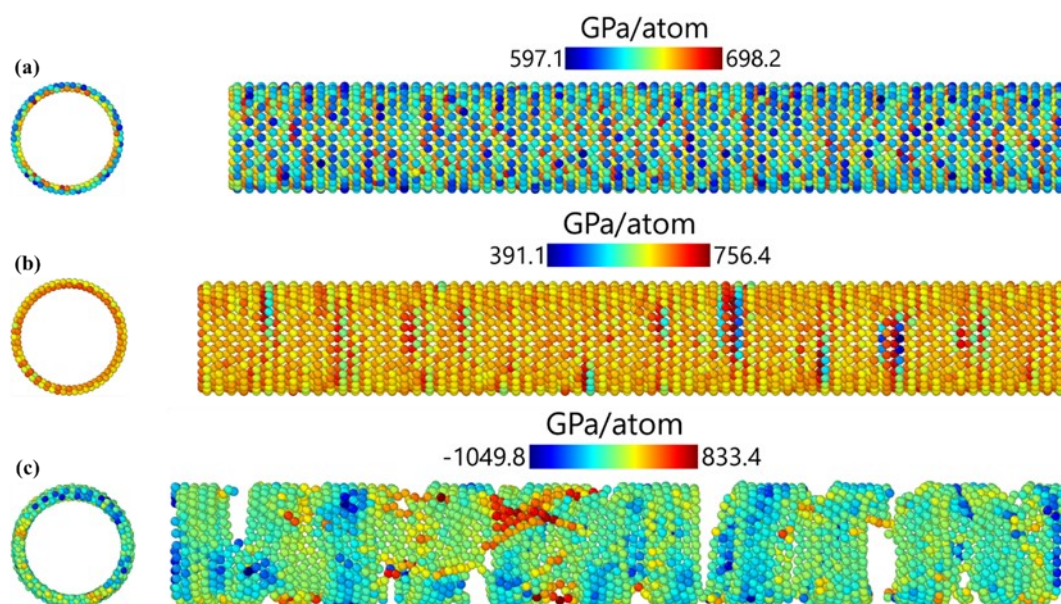


Figure S3. Axial stress distribution of zigzag β -SbNT specimen for the strain states of (a) 28%, (b) 29%, and (c) 30% at 1 K temperature.

Table S1. Numerical values for a number of mechanical properties of all configurations calculated at seven various temperatures.

Structure	Temperature (K)	Ultimate Tensile Stress [GPa·nm] [N/m]	Ultimate Tensile Strain – Fracture Strain	Young's Modulus [GPa·nm] [N/m]
AC α -SbNT	1	7.5072	0.28408	55.0218
	100	7.2459	0.24616	54.9366
	200	6.9035	0.22183	53.9338
	300	6.6916	0.21053	52.8272
	400	6.3711	0.19604	51.8775
	500	6.1206	0.18876	50.8502
	600	5.8216	0.17599	50.6209
ZZ α -SbNT	1	4.9596	0.38389	15.7519
	100	4.3056	0.30363	15.7301
	200	3.8576	0.26859	15.7108
	300	3.6236	0.25162	15.2148
	400	3.2429	0.22905	14.7702
	500	3.0758	0.22038	13.9409
	600	2.5163	0.18325	13.8533
AC β -SbNT	1	7.7980	0.33583	37.9646
	100	7.5671	0.29357	37.6773
	200	7.2344	0.26265	37.5462
	300	7.0757	0.25756	37.5123
	400	6.6850	0.23363	36.7502
	500	6.3442	0.21539	35.9086
	600	6.0533	0.20363	35.8677
ZZ β -SbNT	1	8.4483	0.28773	38.9055
	100	8.1143	0.25681	38.6301
	200	7.7428	0.23667	38.0087
	300	7.3568	0.22122	37.5418
	400	7.1117	0.21336	37.3862
	500	7.0349	0.21173	36.7593
	600	6.2883	0.18551	36.5950

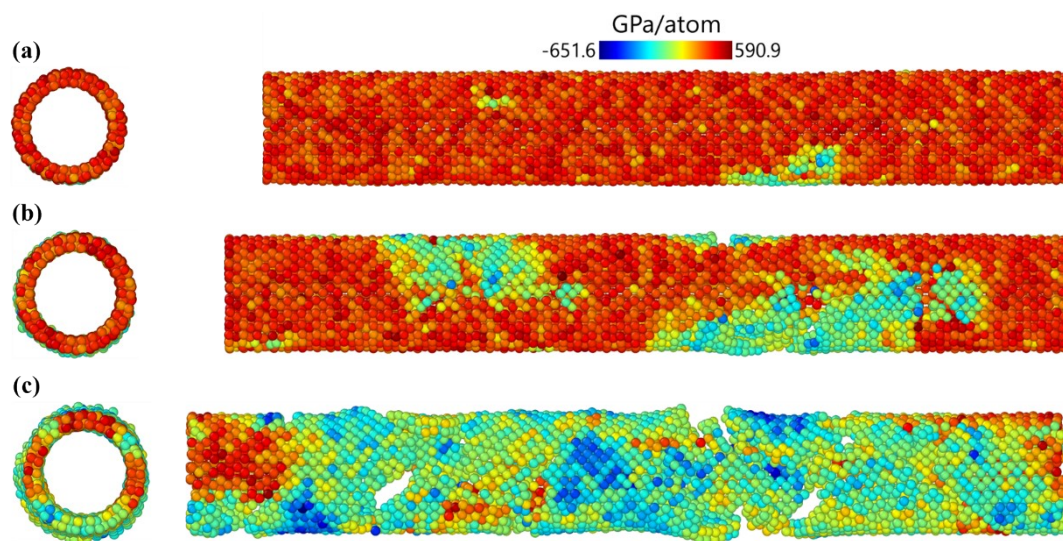


Figure S4. Axial stress distribution of armchair α -SbNT specimen for the strain states of (a) 21%, (b) 22%, and (c) 23% at 300 K temperature.

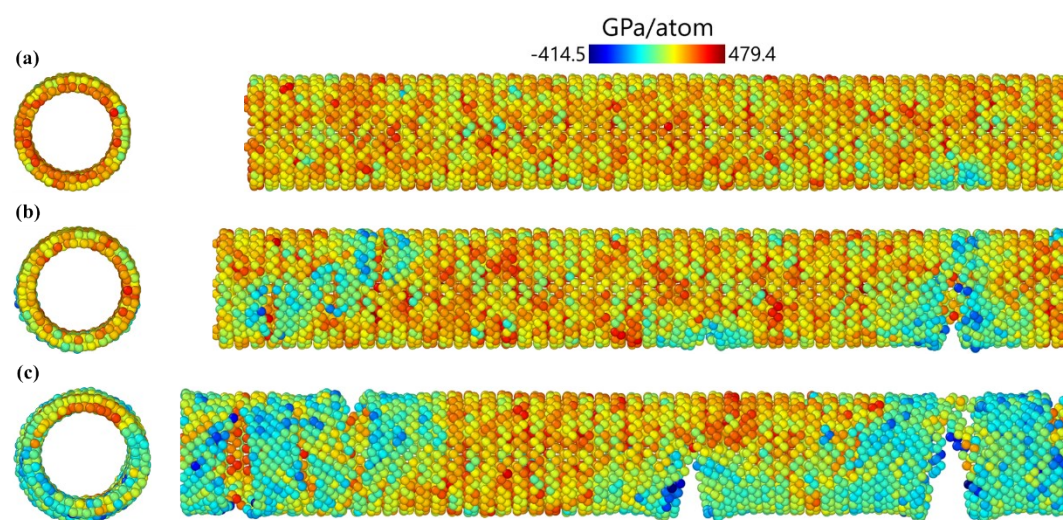


Figure S5. Axial stress distribution of zigzag α -SbNT specimen for the strain states of (a) 26%, (b) 27%, and (c) 28% at 300 K temperature.

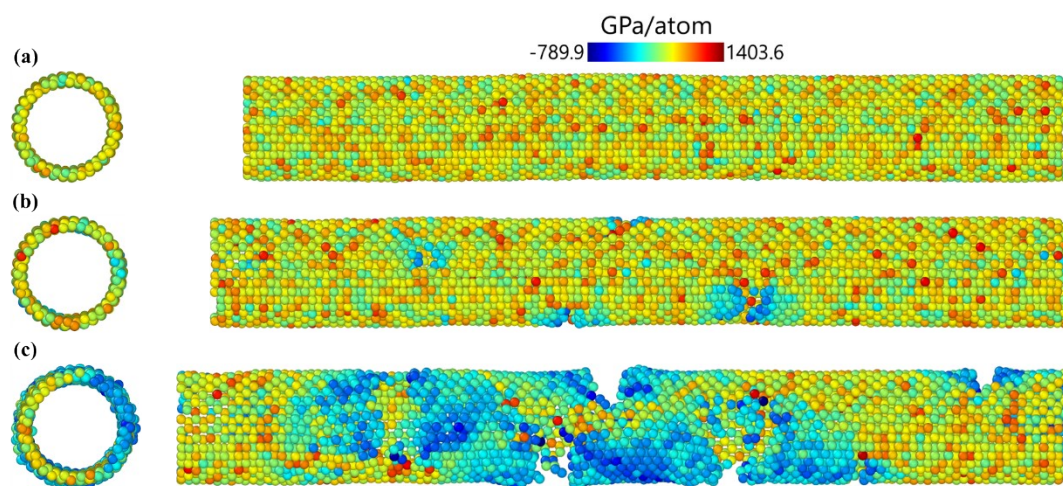


Figure S6. Axial stress distribution of armchair β -SbNT specimen for the strain states of (a) 25%, (b) 26%, and (c) 27% at 300 K temperature.

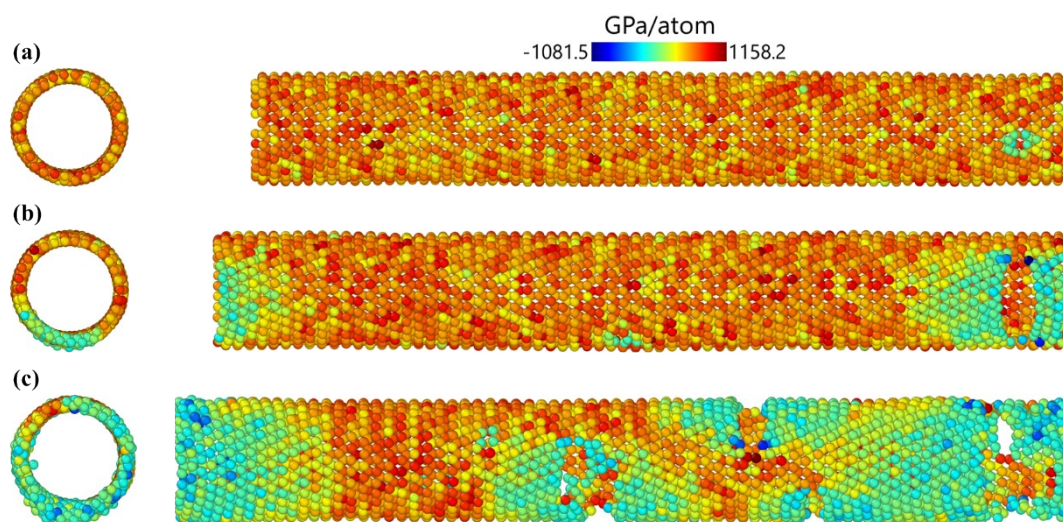


Figure S7. Axial stress distribution of zigzag β -SbNT specimen for the strain states of (a) 22%, (b) 23%, and (c) 24% at 300 K temperature.

Table S2. Numerical values for a number of mechanical properties of all configurations calculated at seven various diameters.

Structure	Diameter (Å)	Length (Å)	Aspect Ratio	Ultimate Tensile Stress [GPa·nm] [N/m]	Ultimate Tensile Strain – Fracture Strain	Young's Modulus [GPa·nm] [N/m]
AC α -SbNT	29.9415	180.9400	6.04312	6.2771	0.2061	51.2231
	35.9646	215.8200	6.00090	6.4748	0.2055	52.6375
	41.9875	250.7000	5.97082	6.6916	0.2105	52.8272
	44.9989	272.5000	6.05570	6.4589	0.1923	53.2419
	51.0216	307.3800	6.02451	6.7607	0.2081	53.3036
	54.0330	329.1800	6.09220	6.7779	0.2053	53.4302
	60.0556	359.7000	5.98945	6.8706	0.2094	53.9344
ZZ α -SbNT	30.6008	187.2512	6.11916	2.8596	0.2138	13.0881
	34.7643	206.1712	5.93054	3.2018	0.2315	14.3133
	41.7034	253.4712	6.07795	3.6236	0.2516	15.2148
	45.8669	281.8512	6.14498	3.6763	0.2530	15.6558
	50.0304	300.7712	6.01177	3.5686	0.2377	15.9170
	55.5817	338.6112	6.09213	3.8092	0.2561	16.2929
	59.7452	357.5312	5.98427	3.8000	0.2516	16.3770
AC β -SbNT	30.9432	187.4600	6.05820	7.0718	0.2664	36.6241
	35.5178	216.3000	6.08990	6.8880	0.2438	36.8930
	40.2564	249.2600	6.19181	7.0727	0.2576	37.5123
	44.7994	269.8600	6.02374	7.0970	0.2558	37.6486
	49.3423	298.7000	6.05363	7.1510	0.2577	37.6759
	56.1567	335.7800	5.97934	7.2420	0.2606	37.7254
	60.6997	360.5000	5.93907	7.2647	0.2595	37.7599
ZZ β -SbNT	30.4929	183.1586	6.00660	7.3531	0.2319	37.3156
	35.7387	218.8388	6.12330	7.5192	0.2344	37.5118
	40.9844	247.3830	6.03603	7.3568	0.2212	37.5418
	44.9187	268.7912	5.98395	7.5326	0.2279	37.9641
	50.1645	304.4714	6.06946	7.5353	0.2264	38.2546
	55.4102	333.0156	6.01001	7.5140	0.2229	38.4494
	60.6560	361.5598	5.96082	7.5785	0.2256	38.7213