

Tunable ductility of a nano-network from few-layered graphene bonded with benzene: A molecular dynamics study

The detailed information of critical strains and stresses for all the models mentioned in the text are given in Table S1.

Table S1 The critical strains and stresses in stretching direction of the samples under the strain rate of 0.1%/ps at different temperatures. “Pristine GN” means pristine graphene ribbon. “1st σ ” is first peak value of x-stress, and “1st ϵ_c ” is the first critical value of x-strain with respect to breakage of surface layers. “2nd ϵ_c ” is the second critical value with respect to thorough breakage of all the layers.

T	Pristine GN		P3C2 model			P3C3 model			
	ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c
8K	27.0%	33.98	19.1%	22.70	28.6%	28.2	19.1%	24.7	28.9%
50K	25.0%	32.69	19.1%	20.61	26.5%	28.0	19.0%	23.1	26.9%
100K	23.8%	31.62	18.5%	20.03	25.8%	27.0	19.2%	22.1	26.7%
200K	23.1%	29.46	17.4%	19.38	25.2%	25.3	18.1%	20.6	25.4%
300K	21.7%	26.22	16.4%	18.12	24.6%	22.4	16.6%	21.0	25.7%
500K	18.5%	19.66	13.6%	15.95	23.2%	14.2	12.9%	17.2	23.3%
T	Pristine GN		P4C2 model			P4C3 model			
	ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c
8K	27.0%	26.2	18.4%	22.5	32.2%	20.2	17.4%	24.6	32.2%
50K	25.0%	26.3	19.2%	22.8	33.1%	19.5	18.7%	24.3	33.1%
100K	23.8%	25.2	18.2%	23.1	33.3%	18.0	17.3%	22.7	31.4%
200K	23.1%	22.8	16.7%	21.0	31.0%	15.4	16.5%	21.7	30.1%
300K	21.7%	18.7	14.5%	20.2	30.1%	13.9	14.9%	22.1	30.5%
500K	18.5%	16.1	12.8%	17.7	28.3%	12.1	13.0%	14.1	24.8%
T	Pristine GN		P5C2 model			P5C3 model			
	ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c
8K	27.0%	22.4	19.2%	23.3	37.9%	16.3	19.1%	24.9	37.6%
50K	25.0%	21.7	17.8%	23.7	37.7%	15.8	18.0%	25.2	37.4%
100K	23.8%	21.3	17.5%	23.7	37.8%	15.5	17.4%	24.6	36.8%
200K	23.1%	20.1	16.4%	21.4	35.9%	14.4	16.0%	23.9	36.4%
300K	21.7%	18.9	15.1%	21.7	36.2%	13.4	14.6%	19.2	32.4%
500K	18.5%	15.0	11.6%	17.9	33.1%	11.5	12.0%	19.6	32.9%
T	Pristine GN		P6C2 model			P6C3 model			
	ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c	1 st σ /GPa	1 st ϵ_c	2 nd σ /GPa	2 nd ϵ_c
8K	27.0%	22.2	18.7%	23.5	43.3%	16.1	18.5%	23.3	39.6%
50K	25.0%	21.8	18.4%	23.5	43.5%	15.8	18.0%	23.8	40.8%
100K	23.8%	21.2	17.6%	17.4	37.8%	15.0	16.8%	23.9	41.3%
200K	23.1%	20.0	16.2%	21.7	41.3%	14.4	15.9%	20.5	38.8%
300K	21.7%	17.6	13.9%	21.6	41.8%	13.1	14.2%	19.5	37.6%

500K	18.5%	16.1	12.6%	17.9	38.0%	10.6	11.1%	16.0	33.0%
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