Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material

Structure-dependent mechanical properties of self-folded two-dimensional nanomaterials

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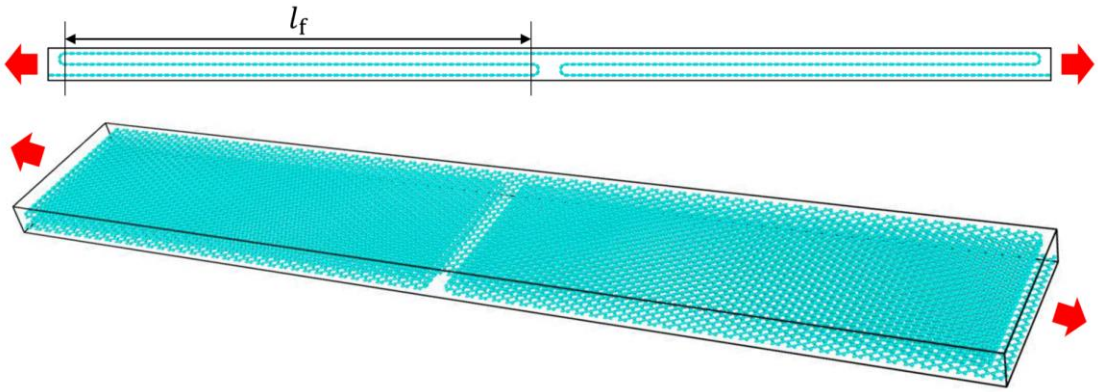

Fig. S1 Atomistic model of MD simulation for uniaxial tension of self-folded graphene.

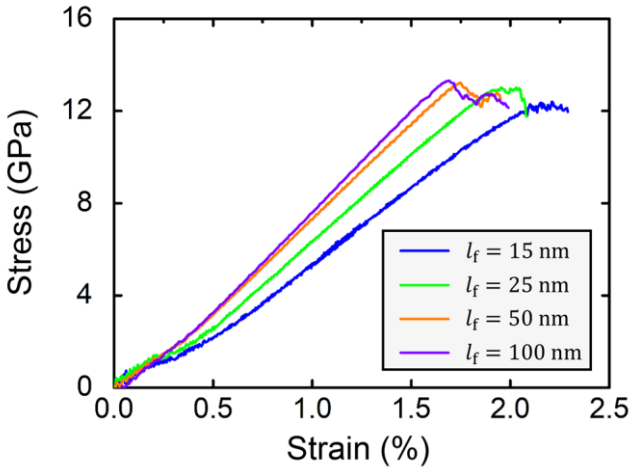

Fig. S2 Stress-strain curves obtained from MD simulations for self-folded graphene under uniaxial tension.

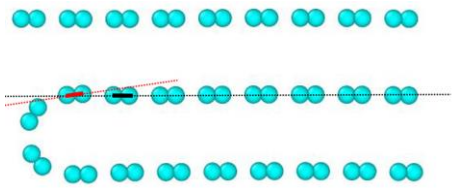

Fig. S3 Local observation of the atomistic model of MD simulation after equilibrium.

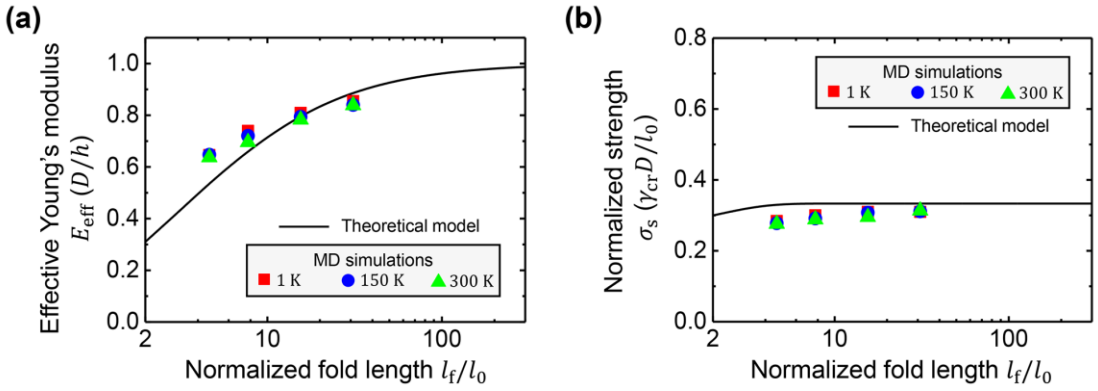

Fig. S4 Effects of temperature on the agreement between the theoretical model and MD simulations. The (**a**) Young's modulus and (**b**) strength with different temperature as 1 K, 150 K and 300 K.

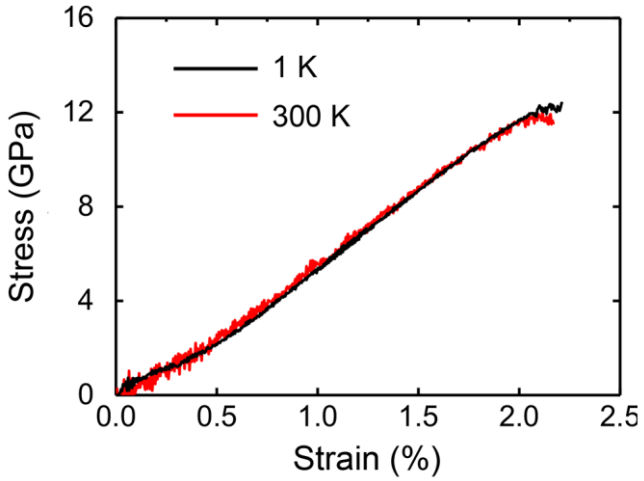

Fig. S5 Comparison of stress-strain curves for simulations under 1 K and 300 K.

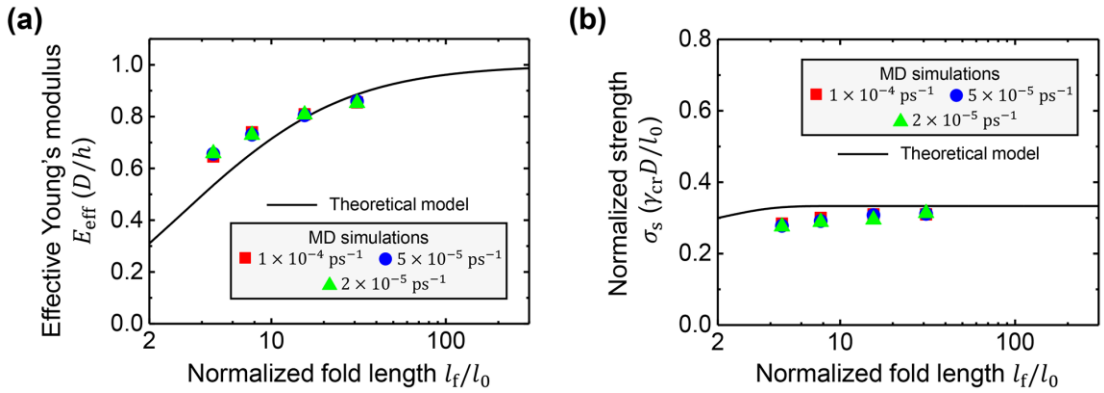

Fig. S6 Effects of strain rate on the agreement between the theoretical model and MD simulations. The (**a**) Young's modulus and (**b**) strength with different strain rates as 1×10^{-4} ps^{-1}, 5×10^{-5} ps^{-1} and 2×10^{-5} ps^{-1}.

Table. S1 Original results of Young's modulus obtained from MD simulations.

	Group 1	Group 2	Group 3	Mean	Standard Deviation	Coefficient of variation
l_f = 15 nm	662 GPa	670 GPa	668 GPa	667 GPa	4.16 GPa	0.624 %
l_f = 25 nm	758 GPa	752 GPa	750 GPa	753 GPa	4.16 GPa	0.553 %
l_f = 50 nm	829 GPa	822 GPa	824 GPa	825 GPa	3.61 GPa	0.437 %
l_f = 100 nm	876 GPa	879 GPa	879 GPa	878 GPa	1.73 GPa	0.197 %

Table. S2 Original results of tensile strength obtained from MD simulations.

	Group 1	Group 2	Group 3	Mean	Standard Deviation	Coefficient of variation
l_f = 15 nm	11.8 GPa	12.3 GPa	12.1 GPa	12.1 GPa	0.262 GPa	2.17 %
l_f = 25 nm	12.5 GPa	12.9 GPa	13.0 GPa	12.8 GPa	0.307 GPa	2.40 %
l_f = 50 nm	12.9 GPa	13.4 GPa	13.5 GPa	13.2 GPa	0.329 GPa	2.48 %
l_f = 100 nm	12.9 GPa	13.7 GPa	13.9 GPa	13.5 GPa	0.551 GPa	4.09 %