Supporting Information for: Temperature-dependent adhesion of graphene suspended on a trench

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Cross-section of sheet deposited at $T = 0$

At zero temperature, the detached part of the sheet is not entirely flat in its cross section, and a low-amplitude ripple can be seen. Figure S1 shows a cross-section taken 1.5 nm from the trench edge for a sheet with adhesion $\varepsilon = 0.1$ eV.

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Alternative temperature protocol

In the majority of simulations, we have first deposited and relaxed a sheet on the substrate at $T = 0$ before raising the temperature slowly, as described in the main text. However, we have also tested an alternative protocol in which the sheet is relaxed away from the substrate at $T = 300$ K, then deposited and relaxed, before the temperature is slowly lowered using a Berendsen thermostat, see the included video cool_from_T300.avi. The interaction with the substrate is characterized by $\varepsilon = 0.04$ eV. Measurements are made by averaging over configurations while the sheet is held at constant temperature using a Langevin thermostat. The change in depth is T is consistent with results from the heating protocol, although the absolute depth is smaller, as shown in Fig. S2. The stresses are very similar, as shown in Fig. S3.

Example videos of sheet deposition and fluctuations

We include four videos. In all cases the trench has width 15 nm and edges of radius of curvature $r = 1$ nm, with adhesion $\varepsilon = 0.04$ eV:

- deposition_T0.avi shows the initial relaxation of a sheet deposited at $T = 0$,
- steady-state_T200.avi shows steady state fluctuations at $T = 200$ K,
- steady-state_10T00.avi shows steady state fluctuations at $T = 1000$ K,
- cool_from_T300.avi shows deposition and cooling of a sheet initially at 300 K, with the temperature ramped down to 0.

Role of trench width in the 1d model

We have tested how the depth h of the sheet center varies as the trench width l and sheet length L are simultaneously increased at $T = 0$, for a sheet with width $w = 1.93$ μm (based on the system studied experimentally by Bunch *et al*[1]). We find the depth grows sublinearly with L.

Resonance frequency of large sheets

The fundamental frequency f of a string of length L, mass density m and under tension t is

$$f = \frac{\sqrt{t/m}}{2L}. \tag{1}$$

We calculate this frequency using the $T = 0$ configuration of our 1d model with $\varepsilon = 0.04$ eV. We treat the sheet as a line with $m = w\rho m_C$ where w is the sheet width, ρ the number density of atoms and m_C the mass of a carbon atom. The tension t is calculated from the strain in the detached sheet. Figure S5 shows the calculated f for a range of trench rim radii of curvature r, for a sheet of width 1.93 μm over a trench of width 1.1 μm, values taken from Bunch *et al*'s experimental work.[1] In that work, a resonance frequency of 70.5 MHz was found (Fig. 2B).

References

(1) Bunch, J. S.; van der Zande, A. M.; Verbridge, S. S.; Frank, I. W.; Tanenbaum, D. M.; Parpia, J. M.; Craighead, H. G.; McEuen, P. L. *Science* **2007**, *315*, 490–493

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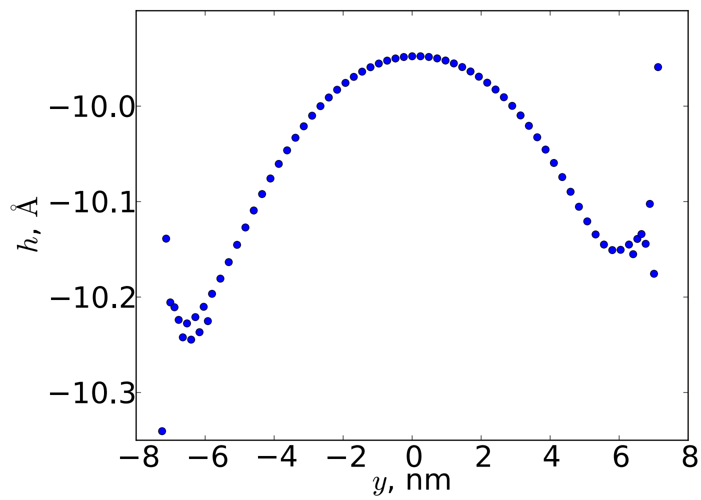

Figure S1: Cross-section taken 1.5 nm from the trench edge for a sheet with adhesion $\varepsilon = 0.1$ eV.

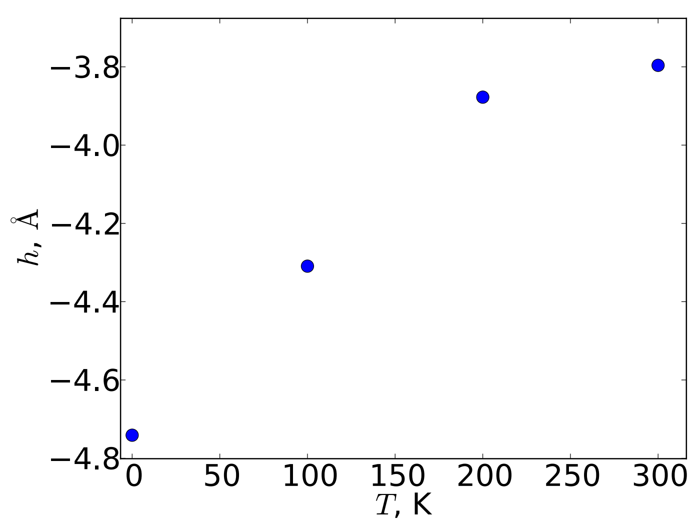

Figure S2: Depth of the center of the sheet, h, plotted against temperature T.

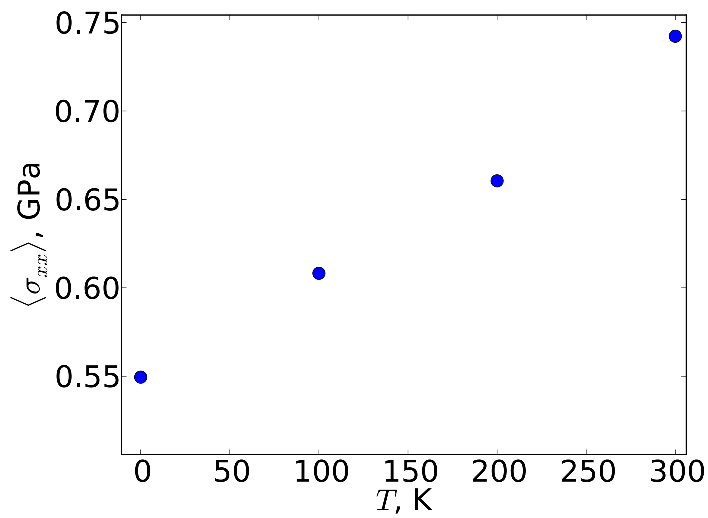

Figure S3: Temperature dependence of the mean stress along the long axis, measured in the sheet center.

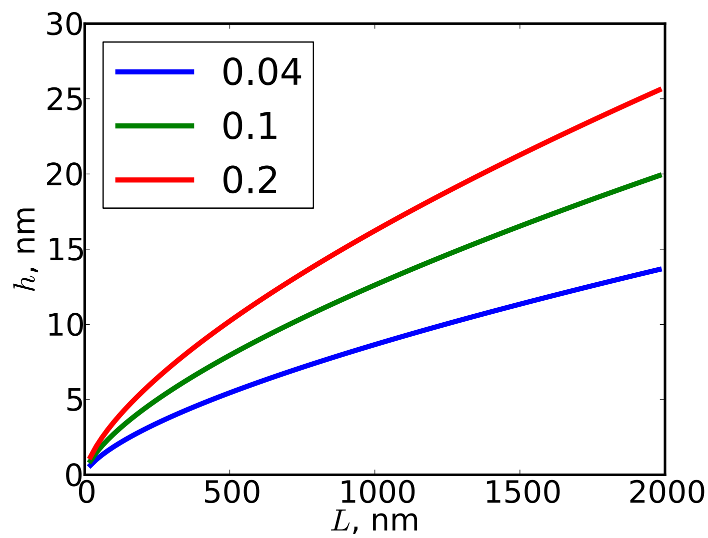

Figure S4: Depth of the sheet center in the 1d model at $T = 0$, in the case $L = l$ and $w = 1.93\ \mu$m, for adhesion ε (in eV) as reported in the legend.

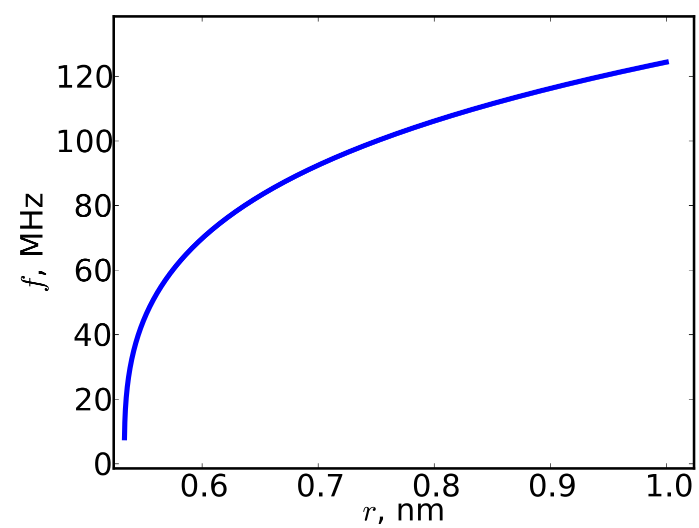

Figure S5: Fundamental frequency f for a sheet of width 1.93 μm suspended over a trench of width 1.1 μm with adhesion energy $\varepsilon = 0.04$ eV, plotted against trench edge curvature r.