

SUPPORTING INFORMATION

Nanomechanical stimulus accelerates and directs the self-assembly of silk-elastin-like nanofibers

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Description of AFM Simulation Approach:

We performed AFM numerical simulations by integrating two coupled differential equations of motion corresponding to the first and second cantilever eigenmodes in order to obtain trajectories of the tip position and tip-sample interaction force as a function of time.¹⁻³ The second cantilever eigenmode was included, as it is known that it can be momentarily excited in liquid environments.¹⁻² This momentary excitation gives rise to additional high-frequency oscillations within each cycle of the fundamental eigenmode, which can have a significant effect on the tip-sample force trajectory.¹⁻² As in the experiments, our simulations used base cantilever excitation. We tracked both the actual tip position and photodetector (cantilever tip slope) readings which have different values for base excitation AFM systems, especially in highly damped environments.⁴ We drove the cantilever using the tapping-mode (amplitude modulation⁵) scheme, controlling the cantilever base position through a proportional-integral loop using either the tip oscillation amplitude or the photodetector amplitude as the feedback parameter. Repulsive tip-sample interactions were introduced through the Derjaguin-Müller-Toporov (DMT) contact model, adopting approximate parameters for tip and sample elasticity corresponding to our experimental system. Attractive interactions were not

included since they are significantly screened in liquid environments.¹⁻² The parameters common to all simulations are summarized in Table S1.

To estimate a range for the maximum tapping force (as opposed to a single value in an ideal steady-state simulation in which every oscillation cycle is identical), we considered AFM control capability, which was quantified through the standard deviation of the experimental amplitude error signal (instantaneous amplitude minus amplitude setpoint) for full scans. Thus, for a given nominal amplitude setpoint we considered various simulations in which the amplitude was set to be equal to different values within the experimentally determined interval, with maximum deviations of three standard deviations from the setpoint in either direction (the values of the base excitation amplitude were selected such that the desired free oscillation amplitude of the tip was obtained). The highest tip-sample forces occurred for the lowest amplitude values in the interval (this is not always true in tapping-mode AFM⁶). As already stated, the standard deviation of the amplitude was determined from the experimental amplitude data by fitting the histogram obtained throughout full 2D scans (such as those shown in Figure 1 of the main manuscript) to a Gaussian function, as illustrated in Figure S1. Examples of typical amplitude control capability in our experiments are provided in Table S2.

Table S1. Parameters used in the AFM simulations

Fundamental cantilever eigenfrequency	14.5 kHz
Second cantilever eigenfrequency	90.625 kHz
Cantilever (base) excitation frequency	14.5 kHz
Fundamental eigenmode force constant	0.003 N/m
Second eigenmode force constant	0.1172 N/m
Fundamental eigenmode quality factor	2
Second eigenmode quality factor	6
Tip and sample Poisson ratio	0.3
Tip modulus of elasticity	130 GPa
Sample modulus of elasticity	2 GPa
Tip radius	10 nm
Oscillation equilibration time	300 fundamental periods (~0.021 ns)

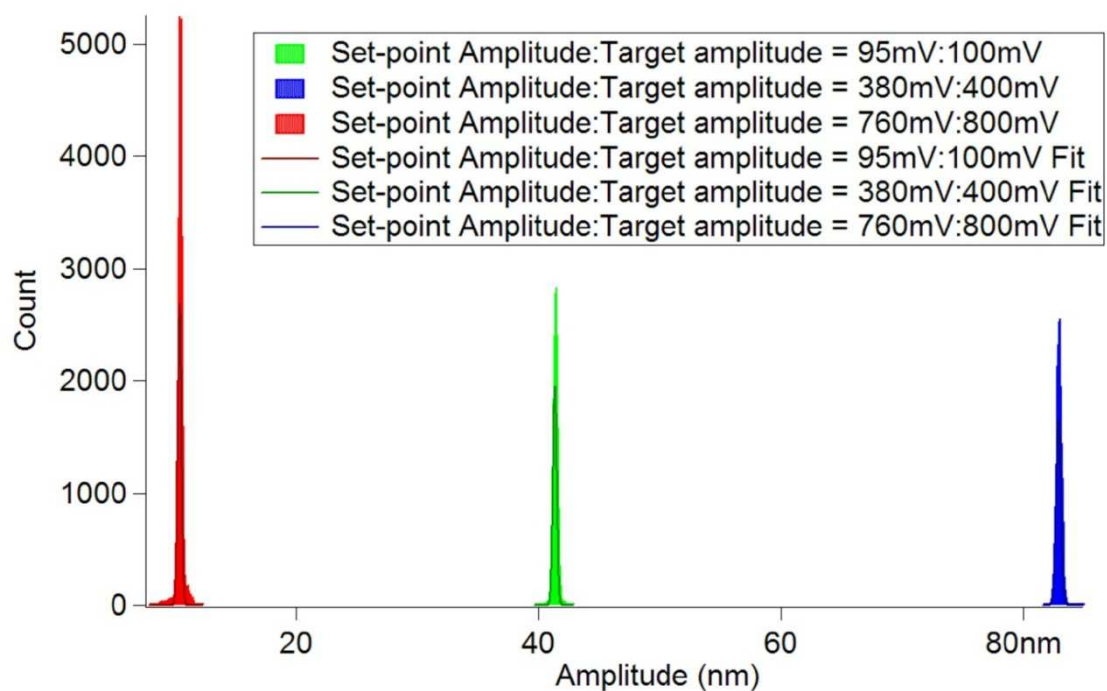


Figure S1. Histogram of amplitude distributions for a few combinations of set-point and free amplitude.

Table S2. Mean amplitude from the photodiode detector for a few typical experiments.

Set-point amplitude (mV): Free amplitude (mV) ^a	Mean Amplitude (nm)	Standard Deviation (nm)
95 : 100	10.42	0.07
380 : 400	41.37	0.07
760 : 800	82.9	0.09

^aThe experimental relationship between the photodiode reading in Volts and the spatial amplitude in nm was obtained through the standard calibration procedure based on measurements of the cantilever deflection (in Volts) for known vertical cantilever displacements (in nm).

Once the amplitude range from the photodiode detector was obtained, a simulation was conducted such that its amplitude was equal to the amplitude setpoint minus three standard deviations. The tip-sample force trajectory obtained was then used to estimate the maximum AFM tapping force. An example of tip and tip-sample force trajectory is provided in Figure S2. The normalized pressure level at each condition (Table S3) was calculated by dividing the maximum tip-sample force observed in the steady state trajectory by the nominal area of the AFM tip used in the experiments, equal to the area of a circle having the same radius as the tip radius of curvature.

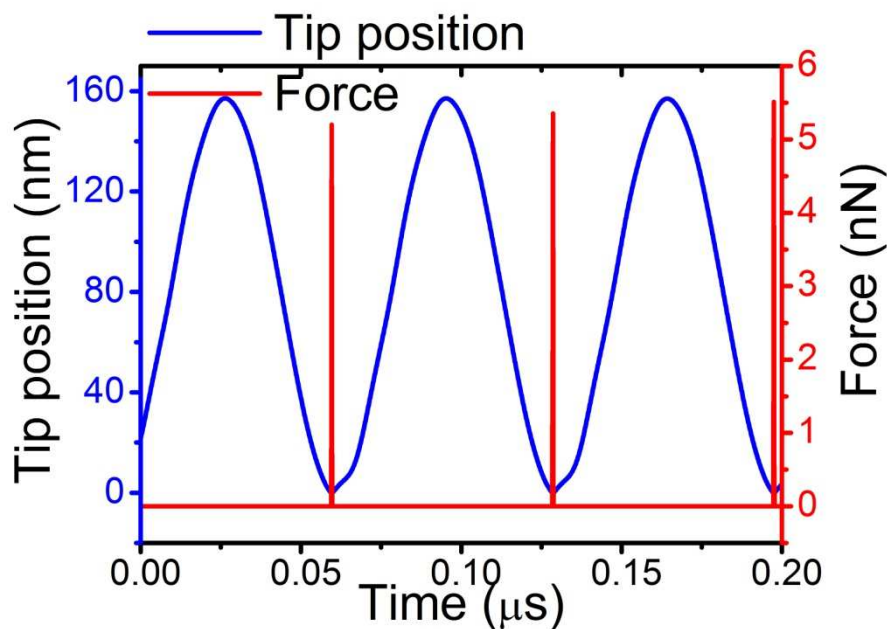


Figure S2. The example of tip trajectory at set-point amplitude : free amplitude ratio equal to 760 mV : 800 mV.

Table S3. Forces and pressures calculated through simulation for a few experimental cases.

Experiment	Simulation			
Setpoint amplitude (mV): Free amplitude (mV)	Average Peak Force (nN)^a	Maximum Peak Force (nN)^b	Average Peak Pressure (MPa)^c	Maximum Peak Pressure (MPa)^d
95 : 100	0.4	0.5	16.4	21.1
380 : 400	2.6	2.9	104	117
760 : 800	5.2	5.5	206	220

^aThis value corresponds to the peak tip-sample force observed throughout the tip trajectory having an amplitude equal to the amplitude setpoint.

^bThis value corresponds to the peak tip-sample force observed throughout the tip trajectory having the lowest amplitude value in the amplitude control interval.

^cThis is the pressure corresponding to the average peak force.

^dThis is the pressure corresponding to the maximum peak force.

References:

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