SI Appendix

Extension per Base Pair for dsDNA used in text

The following formulae compute extension $x(f)$ of a DNA of length h, when a force f is applied at one end of the molecule:

$$\begin{aligned} x(f) &= h\left[1-\frac{1}{\sqrt{4k_{\mathrm{B}}Tfl_p}}\right], \text{ when } 0.08 \text{ pN} < f < 10 \text{ pN}, \\ &= h\left[1-\frac{1}{\sqrt{4k_{\mathrm{B}}Tfl_p}}+\frac{f}{f_0}\right], \text{ when } f > 10 \text{ pN}, \end{aligned}$$

where k_{B} is the Boltzmann constant, l_p is the persistence length of DNA, and f_0 is the stretching elastic constant of the double helix with a numerical value $= 1,000$ pN.

Schiessel *et al.* (1) Model for Nucleosome Diffusion Including Effect of Force

According to the model by Schiessel *et al.* (1), formation of thermally activated intra-nucleosomal loops lead to the repositioning of the nucleosome. The diffusion coefficient of nucleosome at zero force is given by

$$D(0) \approx \frac{k_{\mathrm{B}}T}{\eta l}\left(\frac{\Delta L}{L^*}\right)^2 \exp\left(-\Delta U_0/k_{\mathrm{B}}T\right),$$

where T is the temperature, η is the effective viscosity of the solution, l is the total length of the DNA wrapped around the nucleosome, and L^* is the length of the region on the nucleosome that is exposed when the loop is formed. ΔL is the size of the loop and ΔU_0 is the energy change associated with the formation of the loop at zero force ($f = 0$). ΔU_0 has contributions from the change in curvature energy when the loop is formed as well as the adsorption energy (1). We have used the same numerical values for all the parameters as in ref. 1, except the adsorption energy per unit length. The adsorption energy depends on various factors such as concentration of salt and other charged constituents in the medium. We model experiments in the egg extract and have estimated the value of adsorption energy per unit length as $\approx 42/50\ k_{\mathrm{B}}T/\mathrm{nm}$, noting that the average of the potential is $42\ k_{\mathrm{B}}T$.

The external force modifies ΔU_0 to

$$\Delta U_f = \Delta U_0 + f \cdot \Delta L.$$

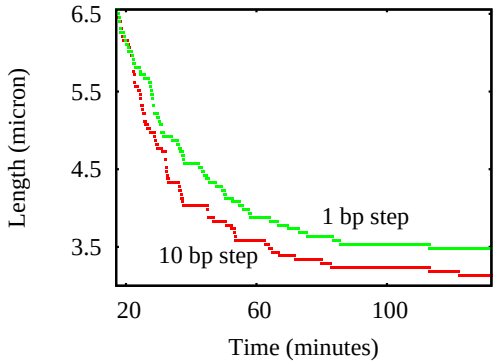

Fig. 4. Comparison of assembly kinetics computed with diffusion using 1-bp step size and 10-bp step size.

This leads to

$$D(f) = D(0) \exp\left(-f\Delta L/k_{\rm B}T\right),$$

Taking $\Delta L = 10$ bp, we get $D(f = 1 \text{ pN}) = 3.2 \times 10^{-15}$ cm^2/s (≈ 3 bp^2/s).

Diffusion Via Twist-Defect Mechanism

It has been also suggested that nucleosomes may slide via 1-bp steps with a twist-defect mechanism (2,3). To test which of the loop or twist-defect mechanisms, is more likely, we have done our Monte-Carlo calculations, with diffusion step size of 1 bp, at a rate of 680 bp^2/s, as suggested by Kulic and Schiessel (3). The results are shown in Fig. 4. The kinetics via 1-bp step diffusion with a rate 680 bp^2/s are much slower than that via 10-bp step diffusion with a rate 5 bp^2/s. The resulting kinetics (via 1-bp step diffusion) do not fit the experimental data. The reason for this slowdown is that the sequence potential highly suppresses diffusion via 1-bp step, as expected in ref. 3.

Fluctuation in the Loop-Diffusion Step Size

We have also generalized our calculations to include small amount of fluctuations in the diffusion (via the loop mechanism) step size as is likely to occur in reality. In the generalized calculations, we choose diffusion step sizes as 9,10, or 11 with equal probabilities, so that the average step size is 10 bp. We find that the kinetics in the new calculation with a rate of $D = 3$ bp^2/s (the number we estimated by using the Schiessel model) is sufficient to explain

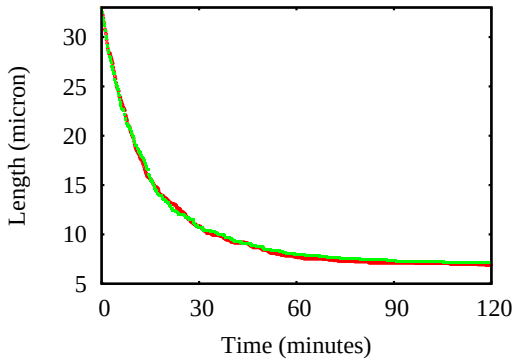

Fig. 5. Kinetics with $D = 3$ bp^2/s in the new calculation (with fluctuating step sizes) compared with $D = 5$ bp^2/s of the calculation with 10-bp step alone.

the experimental data. That is, kinetics with $D = 3$ bp^2/s in the new calculation matches with $D = 5$ bp^2/s of the calculation with 10-bp step alone. This is shown in Fig. 5. This shows that our kinetics are robust for a small fluctuation in the diffusion step sizes.

(1) Schiessel H, Widom J, Bruinsma RF, Gelbart WM (2001) *Phys Rev Lett* 86:4414-4417.

(2) van Holde KE, Yager TD (1985) in *Structure and Function of the Genetic Apparatus*, eds Nicolini C, Ts'o POP (Plenum, New York), pp 35-53.

(3) Kulic IM, Schiessel H (2003), *Phys Rev Lett* 91:148103.