Diffusion, polymers, reptation

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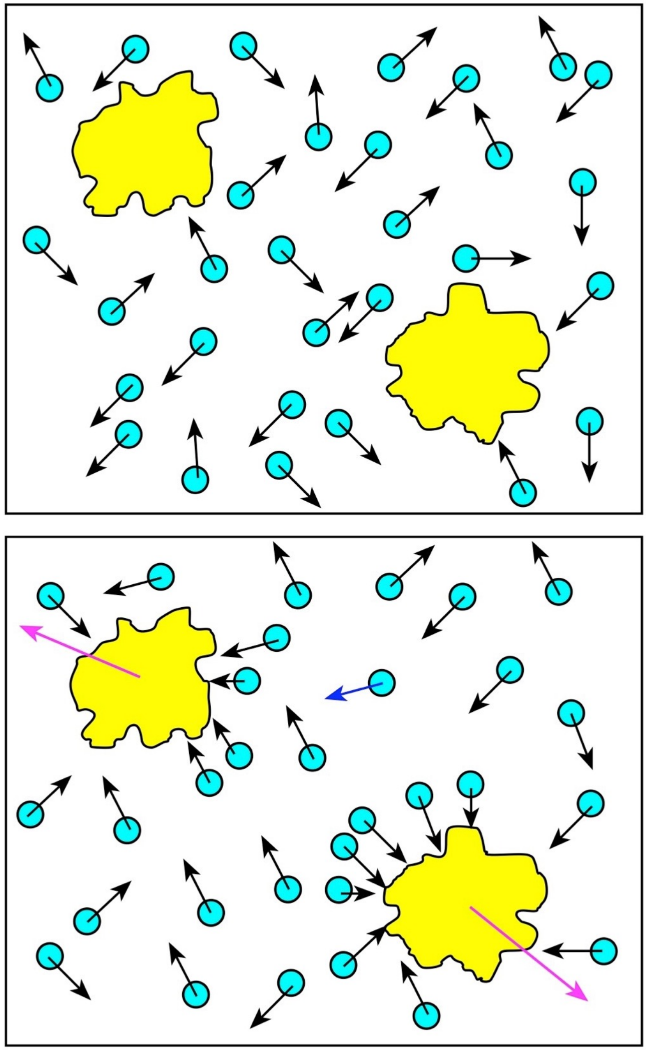
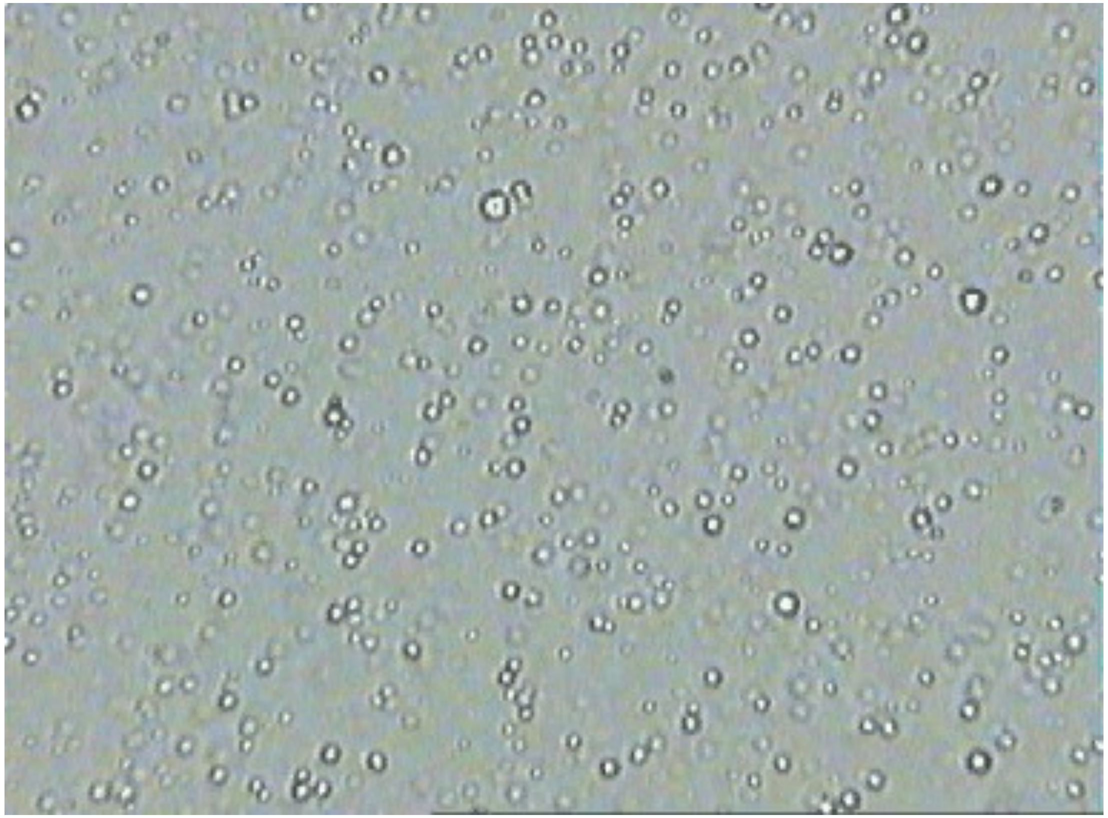
Thermodynamic currents

Differences in the intensive variable at different points in the system induce currents of the conjugate extensive variable.

Thermodynamic current	Intensive quantity	Current density	Law
Heat	Temperature (T)	$J_E = -\lambda \frac{\Delta T}{\Delta x}$	Fourier
Volume	Pressure (p)	$J_V = -\frac{R^2}{8\eta}\frac{\Delta p}{\Delta x}$	Hagen-Poiseuille
Electric current	Electric potential (φ)	$J_Q = -\frac{1}{\rho}\frac{\Delta \varphi}{\Delta x}$	Ohm
Diffusion	Concentration (c)	$J_n = -D\frac{\Delta c}{\Delta x}$	Fick

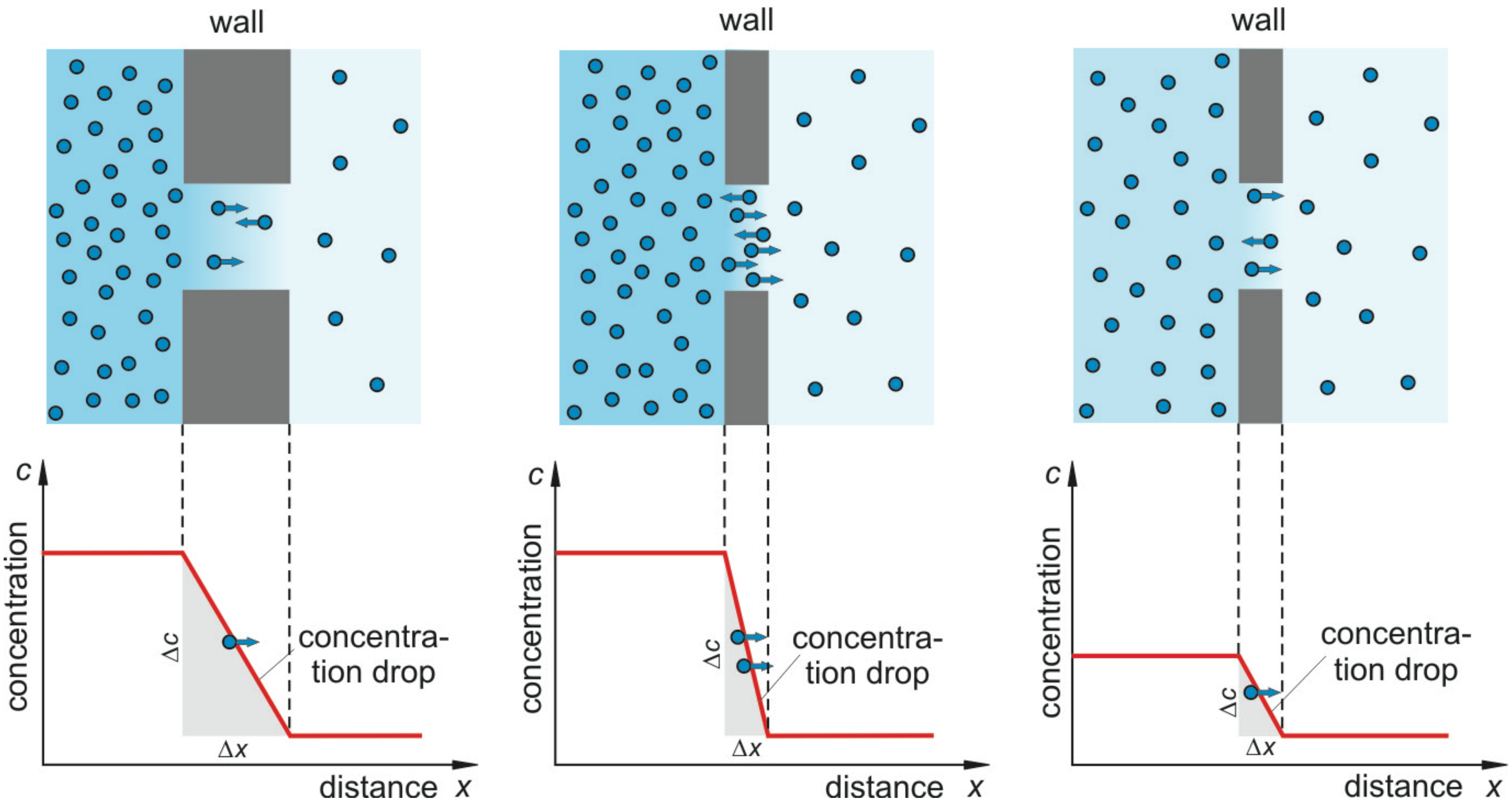
Microscopic background: Brownian motion





Fat droplets in milk
(droplet size 0.5 - 3 µm)

Diffusion


wall
c
concentration
Δc
concentra-
tion drop
Δx
distance x
wall
c
concentration
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tion drop
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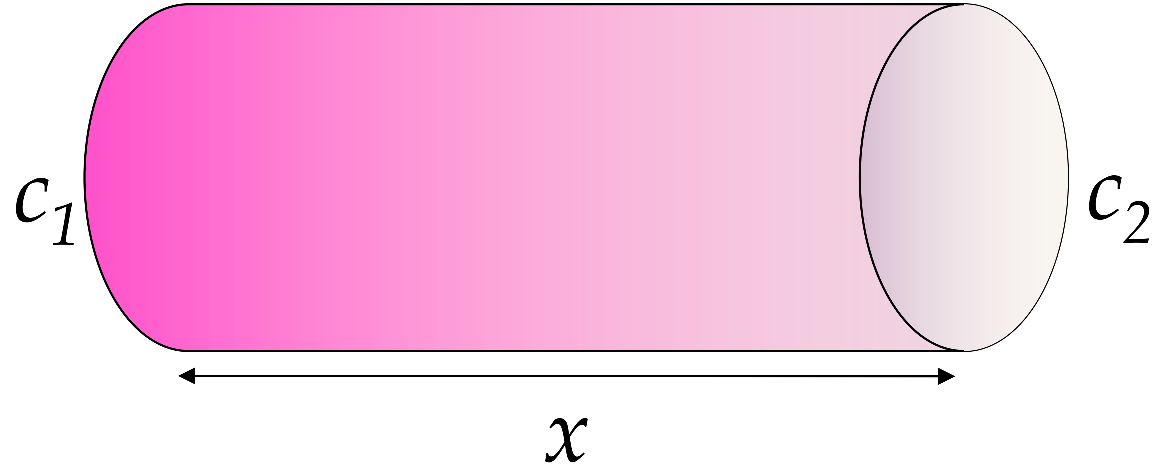
distance x

Fick's first law



$$\frac{m}{tA} = J_n = -D\frac{\Delta c}{\Delta x}$$

m = amount of substance (number of moles)
t = time
x = length
$\Delta c/\Delta x$ = concentration gradient
A = cross section area
J_n = diffusion flux
D = diffusion constant

Thermodynamic currents

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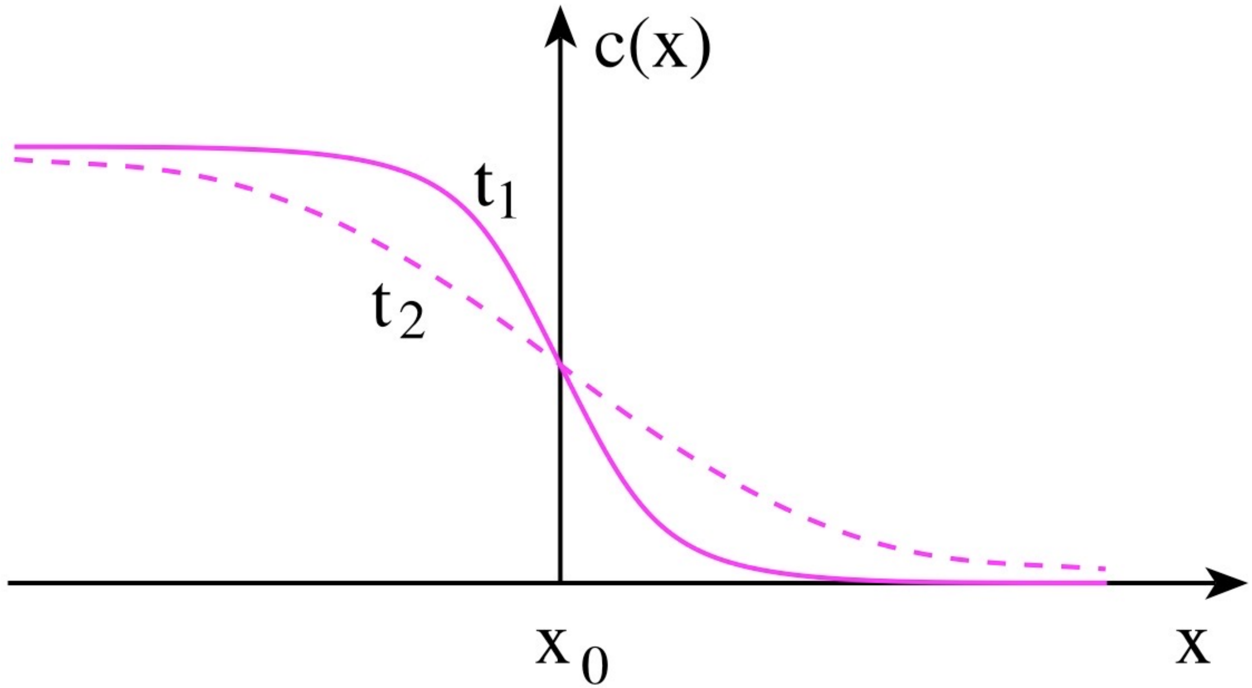
Fick's second law

$$D\frac{\Delta\left(\frac{\Delta c}{\Delta x}\right)}{\Delta x} = \frac{\Delta c}{\Delta t}$$



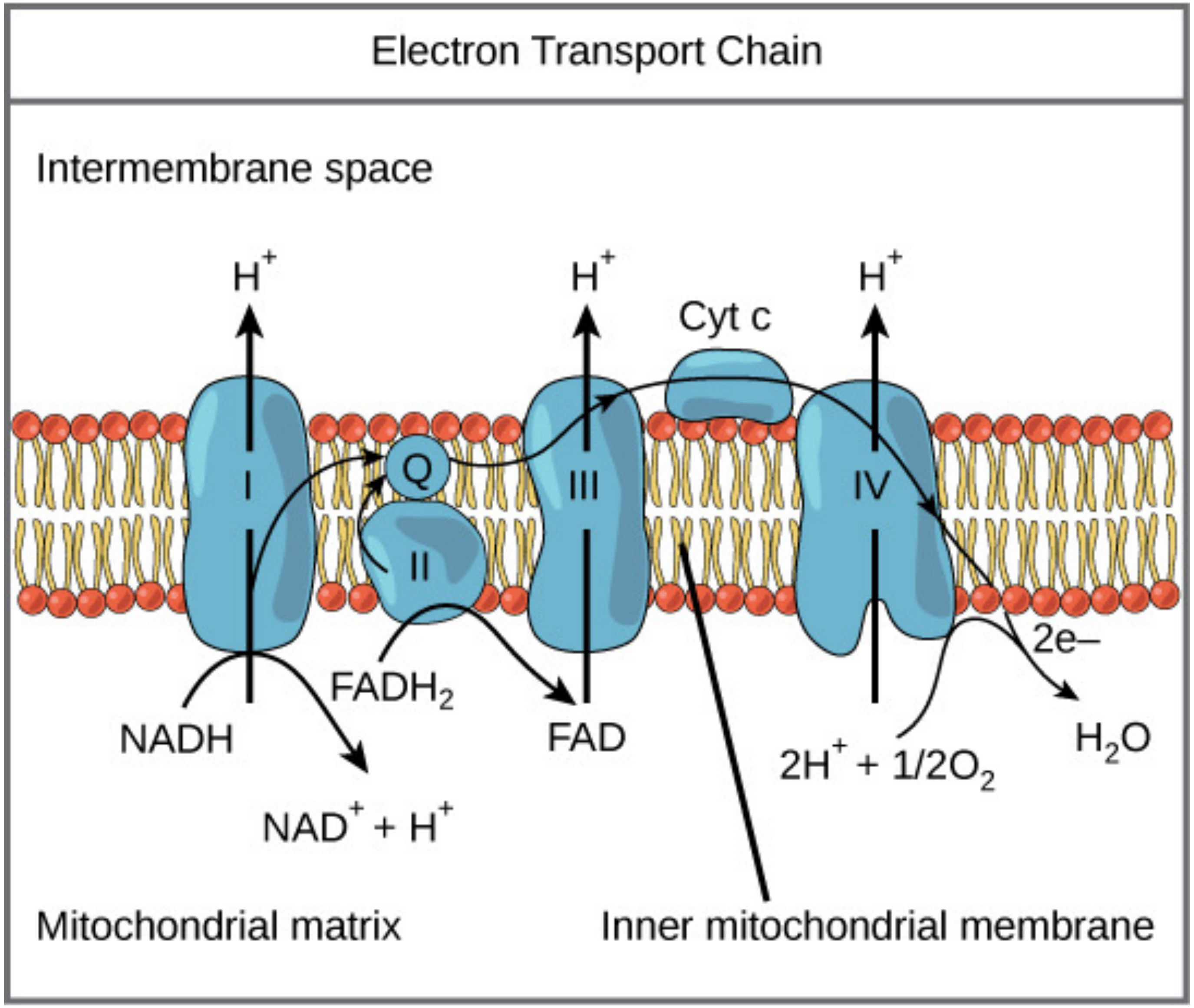
D = diffusion constant

c = concentration

x = distance

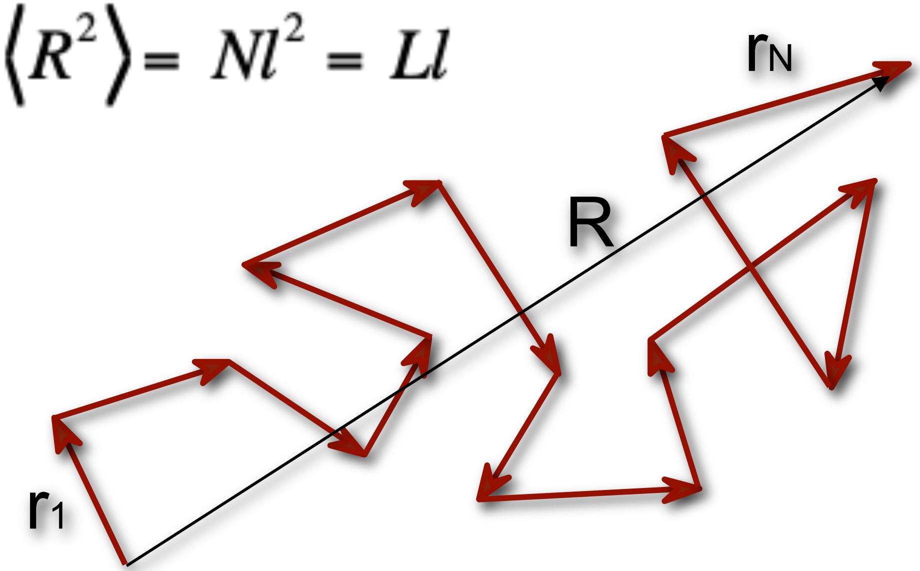
t = time

Directed transport by diffusion



Brownian motion – random walk

$$\langle R^2 \rangle = Nl^2 = Ll$$



R = displacement

N = number of steps

$l = |\vec{r}_i| =$ average free path

r_i = one step

$Nl = L$ = total path

Diffusion constant: $D = \frac{1}{3} v l$

Average particle velocity: $v = \frac{l}{\tau}$

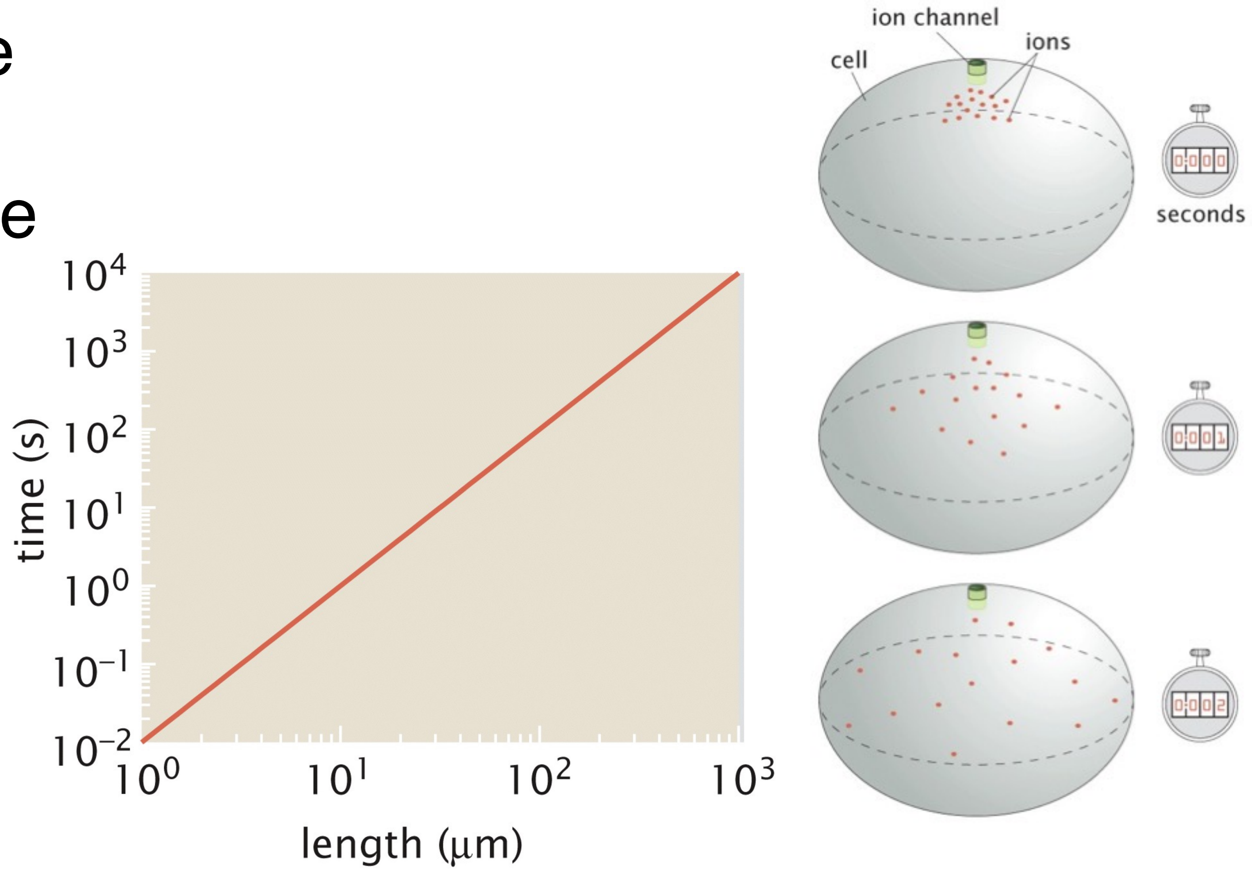
$$\langle R \rangle = \sqrt{Nl^2} = \sqrt{\frac{t}{\tau} l^2} = \sqrt{t v l} = \sqrt{3Dt}$$

The speed of the diffusion

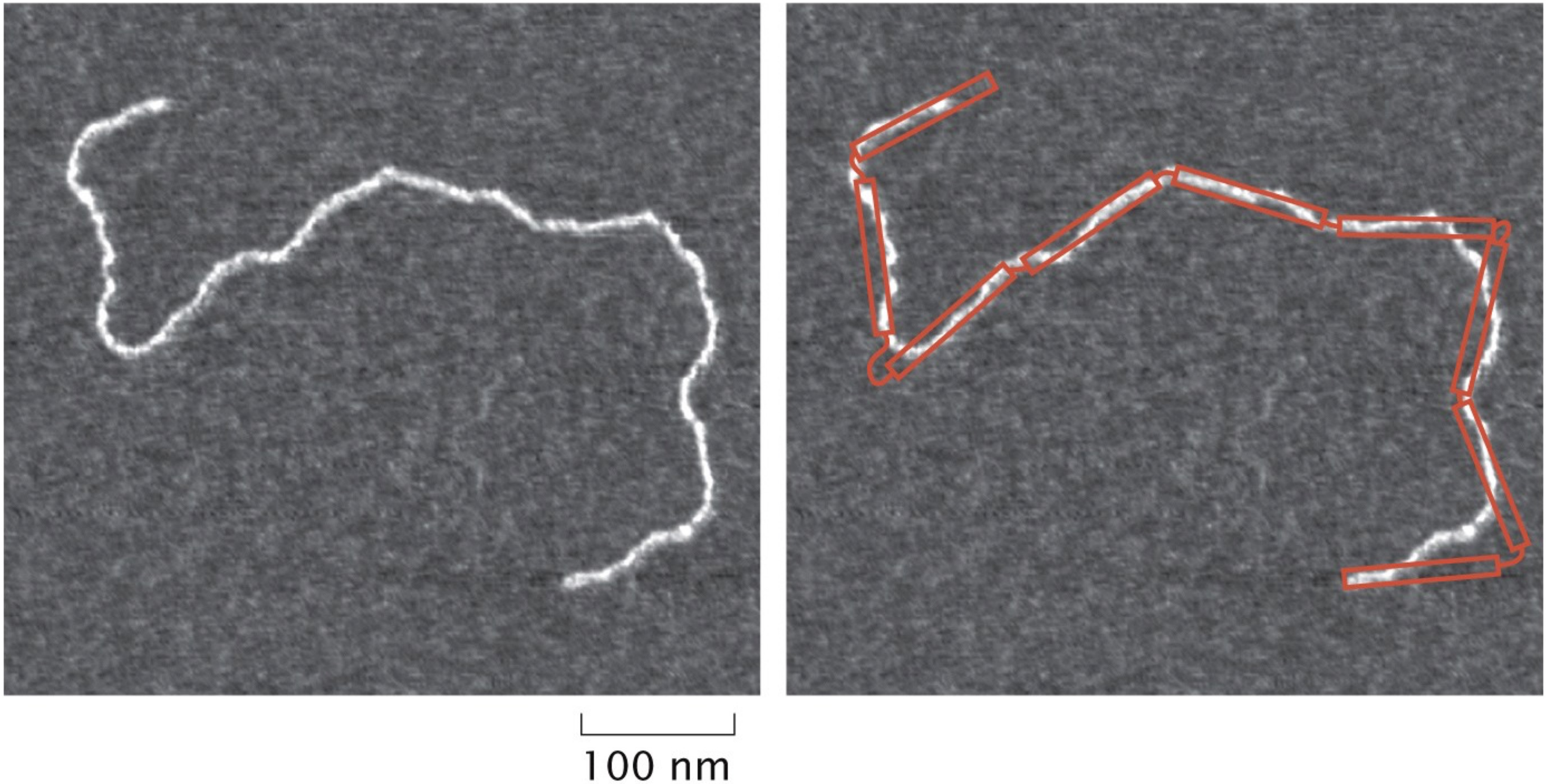
Since the departure of the particles is proportional to the square root of the time, diffusion is

fast on short distances and

slow on long distances.

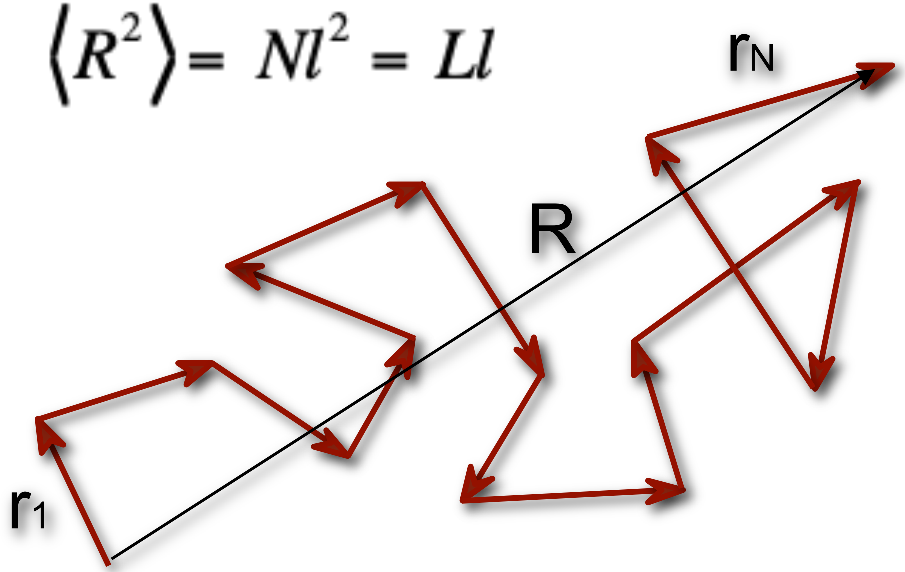


Polymers as random walks

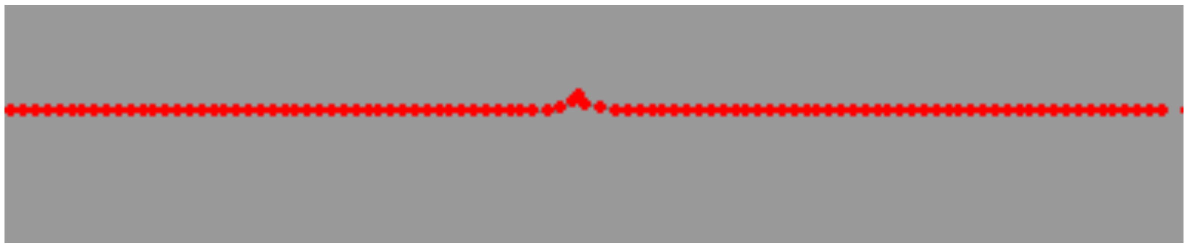


Polymer random walk

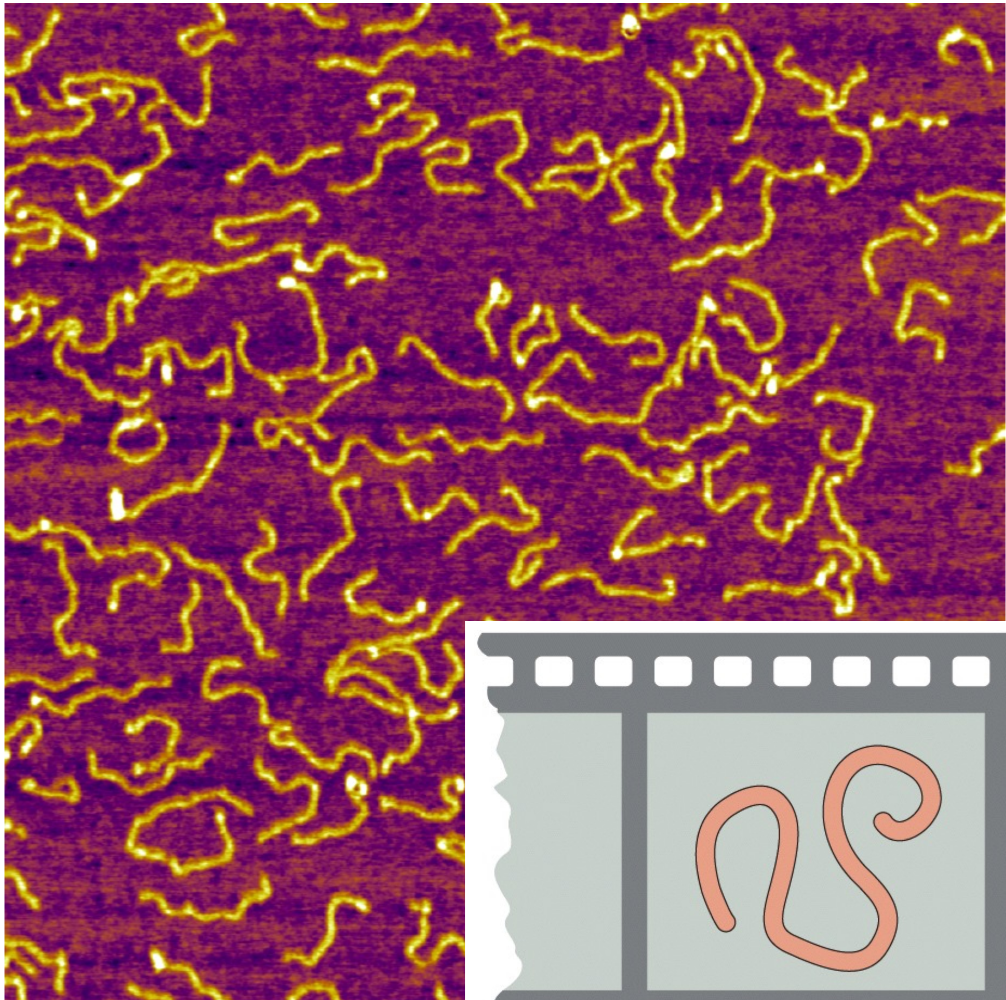
$$\langle R^2 \rangle = Nl^2 = Ll$$



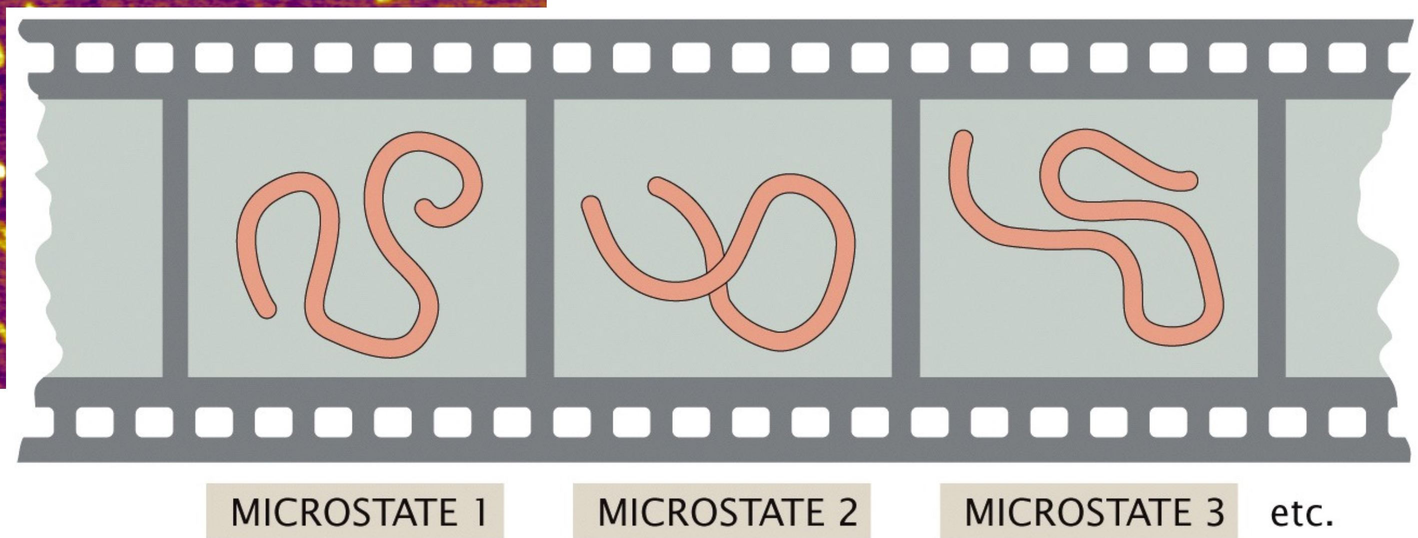
The tendency for elementary vectors to be orientationally disordered results in **elasticity** of the polymer.



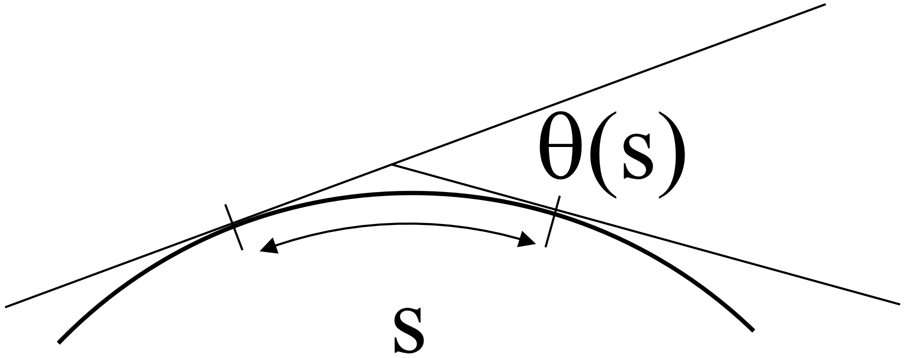
The "equilibrium" state of polymer molecules



The macro state that can be realized with the most micro states (most likely state)



Wormlike chain



$$\langle \cos\theta(s) \rangle = \exp\left(-\frac{s}{l_p}\right)$$

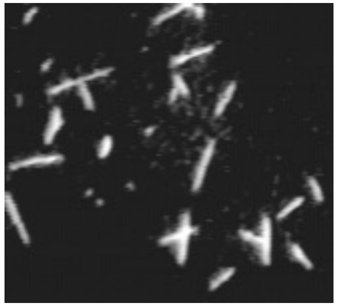
$$l_p = \frac{EI}{k_B T}$$

ℓ_p = persistence length
E = Young's modulus
I = second order moment of the cross section (shape dependent)
$k_B T$ = thermal energy

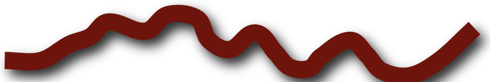
Connection between the shape and persistence length of the polymer

Rigid chain

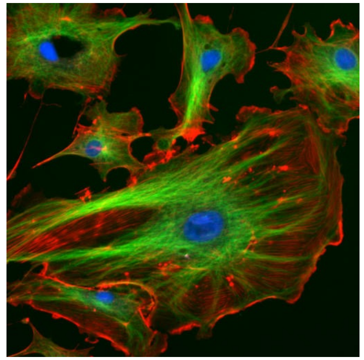
$L_p >> L_c$ Microtubule



Semiflexible chain

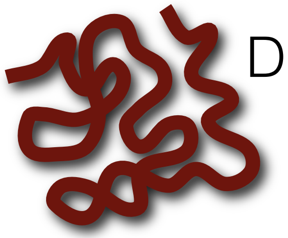


$L_p \approx L_c$ Microfilament (actin)



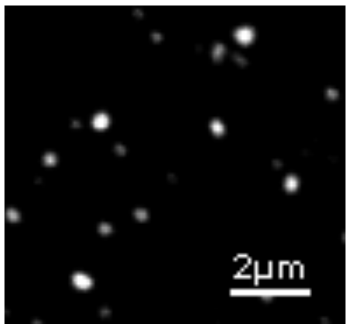
actin
tubulin

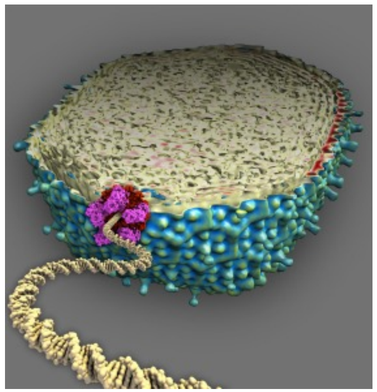
Flexible chain



DNS

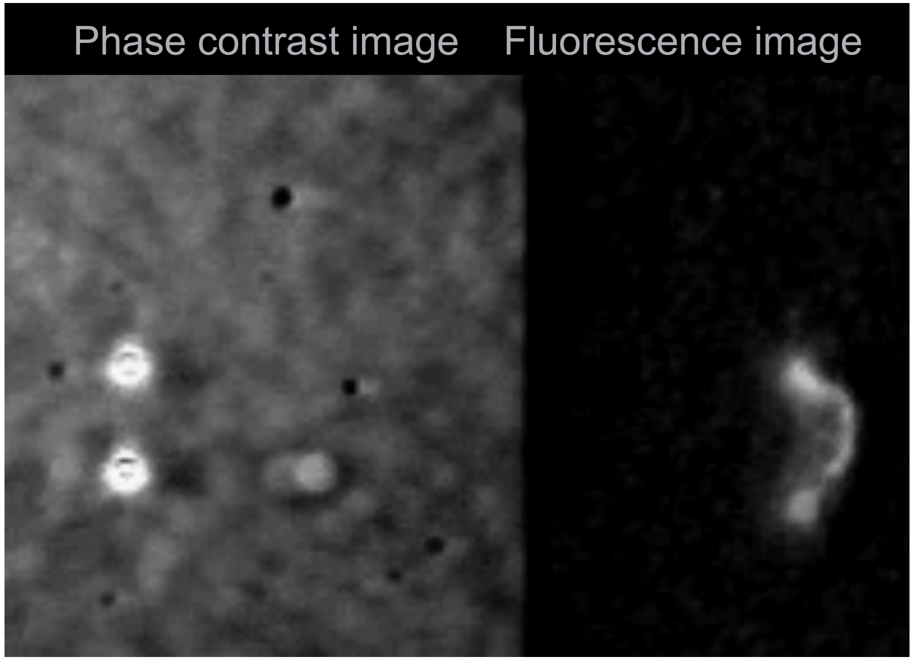
$L_p << L_c$

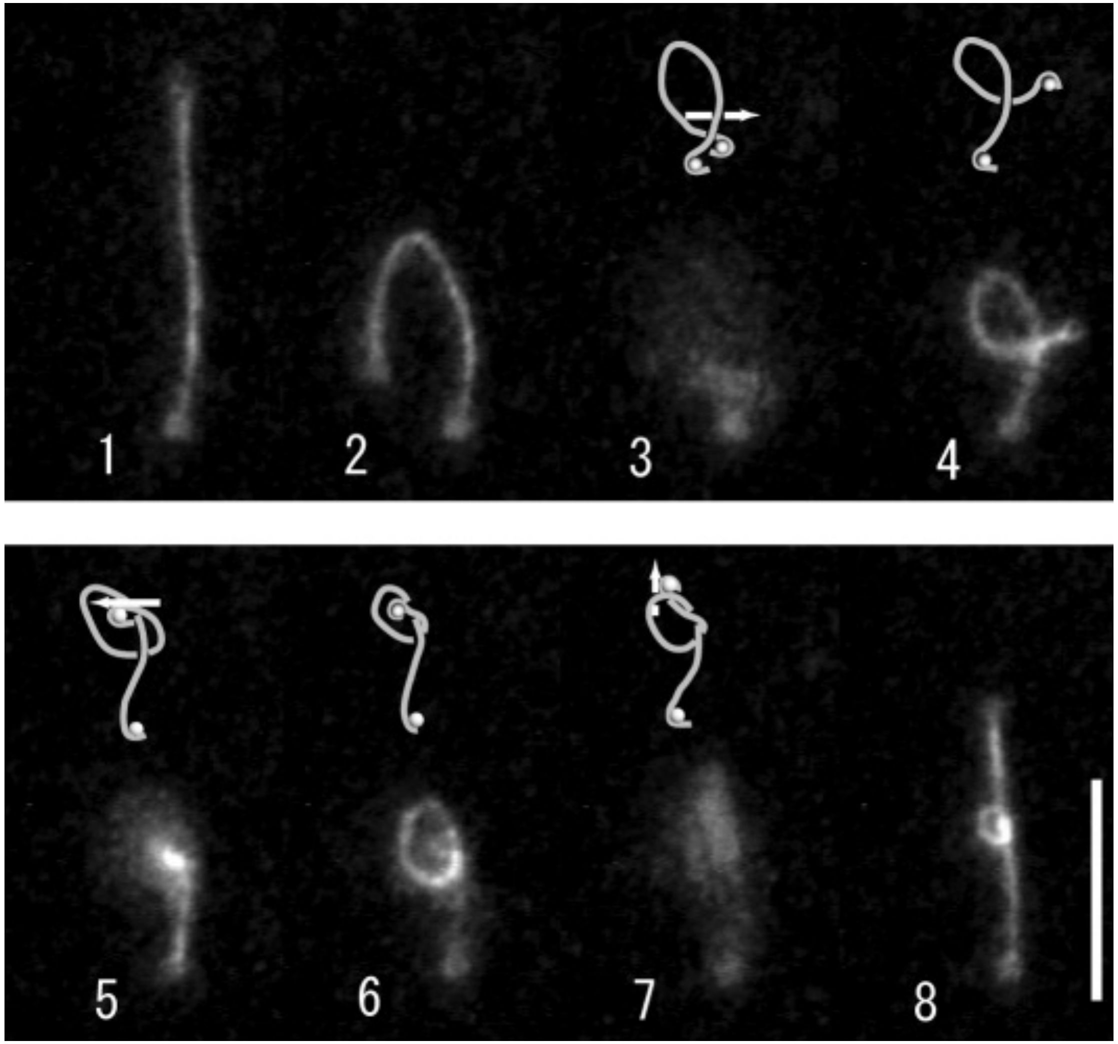




L_p = persistence length, L_c = contour length

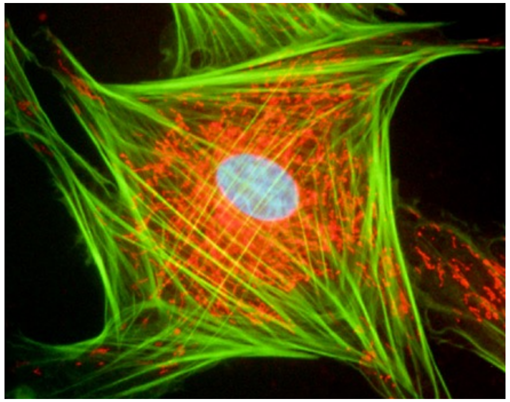
Tying a knot on a DNA molecule using optical trap

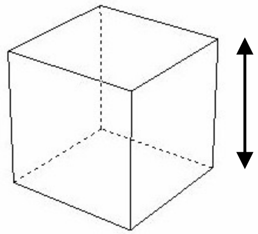




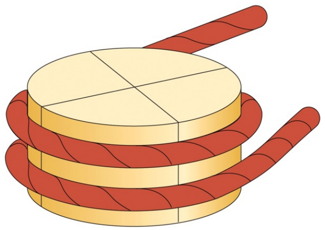
Physical size of the human genome

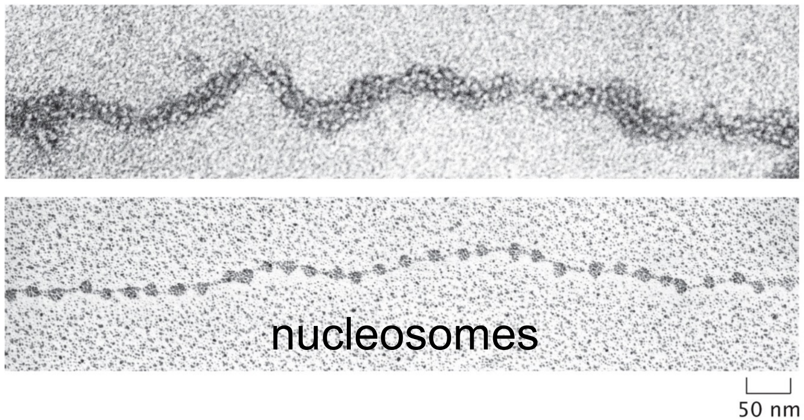
	Idealized cell: 20 μm edge cube	**House:** 20 m edge cube
DNA thickness	2 nm	2 mm
DNA total length	2 m	2000 km
Persistence length	50 nm	5 cm
Average end-to-end distance	320 μm	320 m
Gyration radius (R_G)	130 μm	130 m





20 μm (20 m)



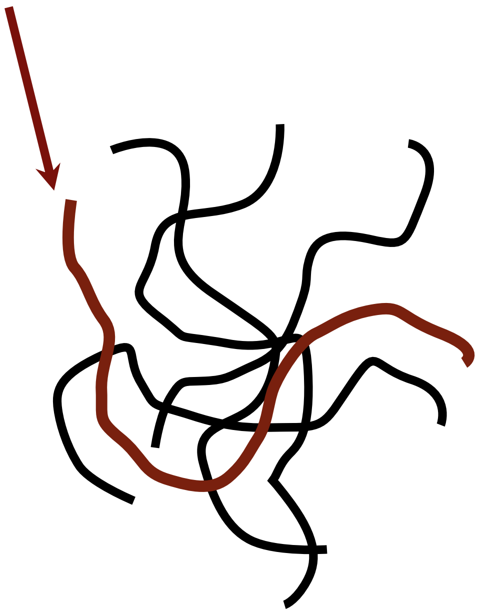


Single nucleosome particle: histone protein octamer + DNA wound ~1.6 x around it

Reptation - a special case of diffusion

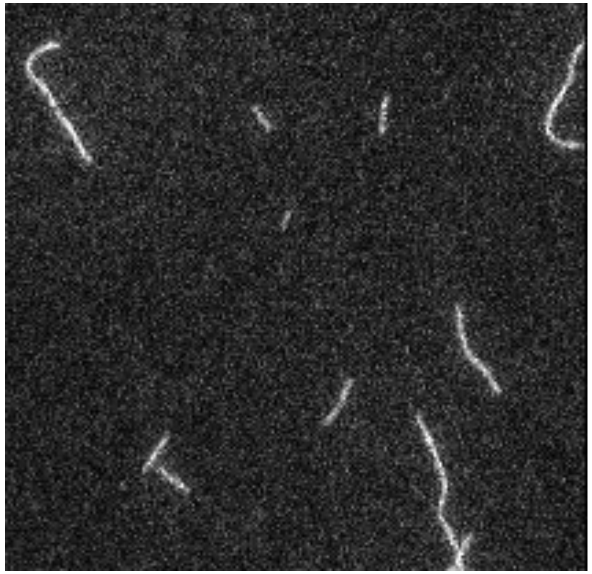
Snake-like diffusion of a polymer in a polymer matrix

Filament in a reptation channel



Indiana Jones and Raiders of the Lost Ark

Actin filaments in metilcelulose matrix



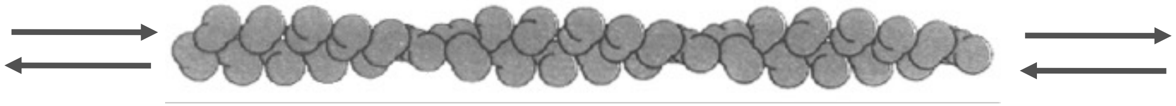
$$\tau_r = \frac{L^2 \cdot N}{\mu \cdot k \cdot T}$$

τ_r - Reptation time

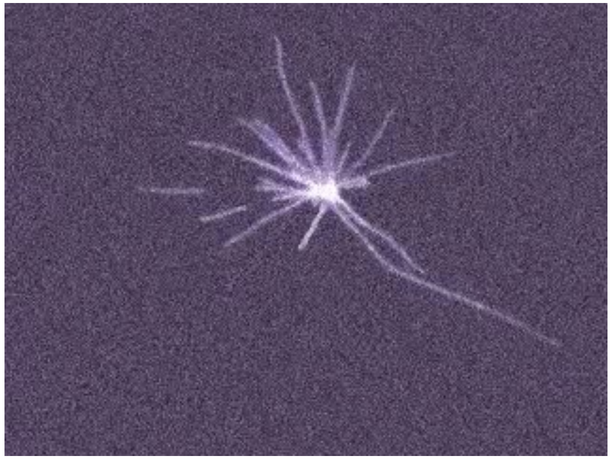
L = contour length
N = number of monomeric units
μ = chain mobility
kT = thermal energy

Polymerization equilibria

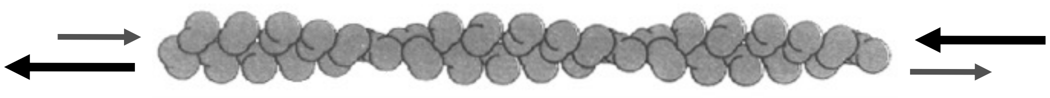
1. True equilibrium

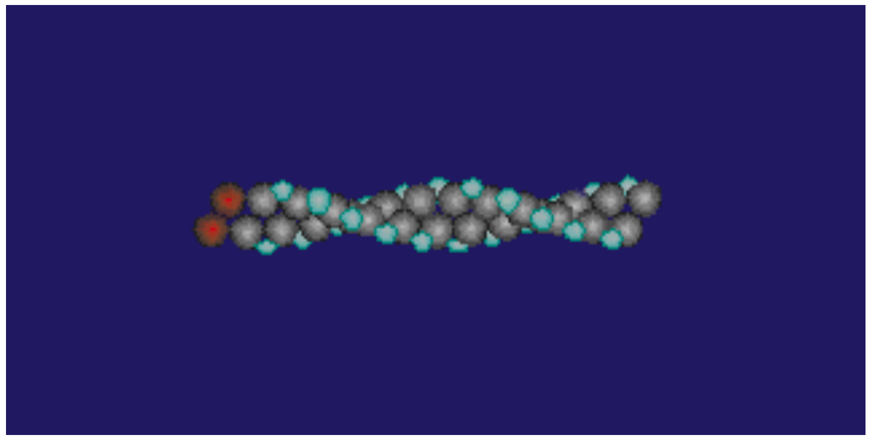


2. Dynamic instability

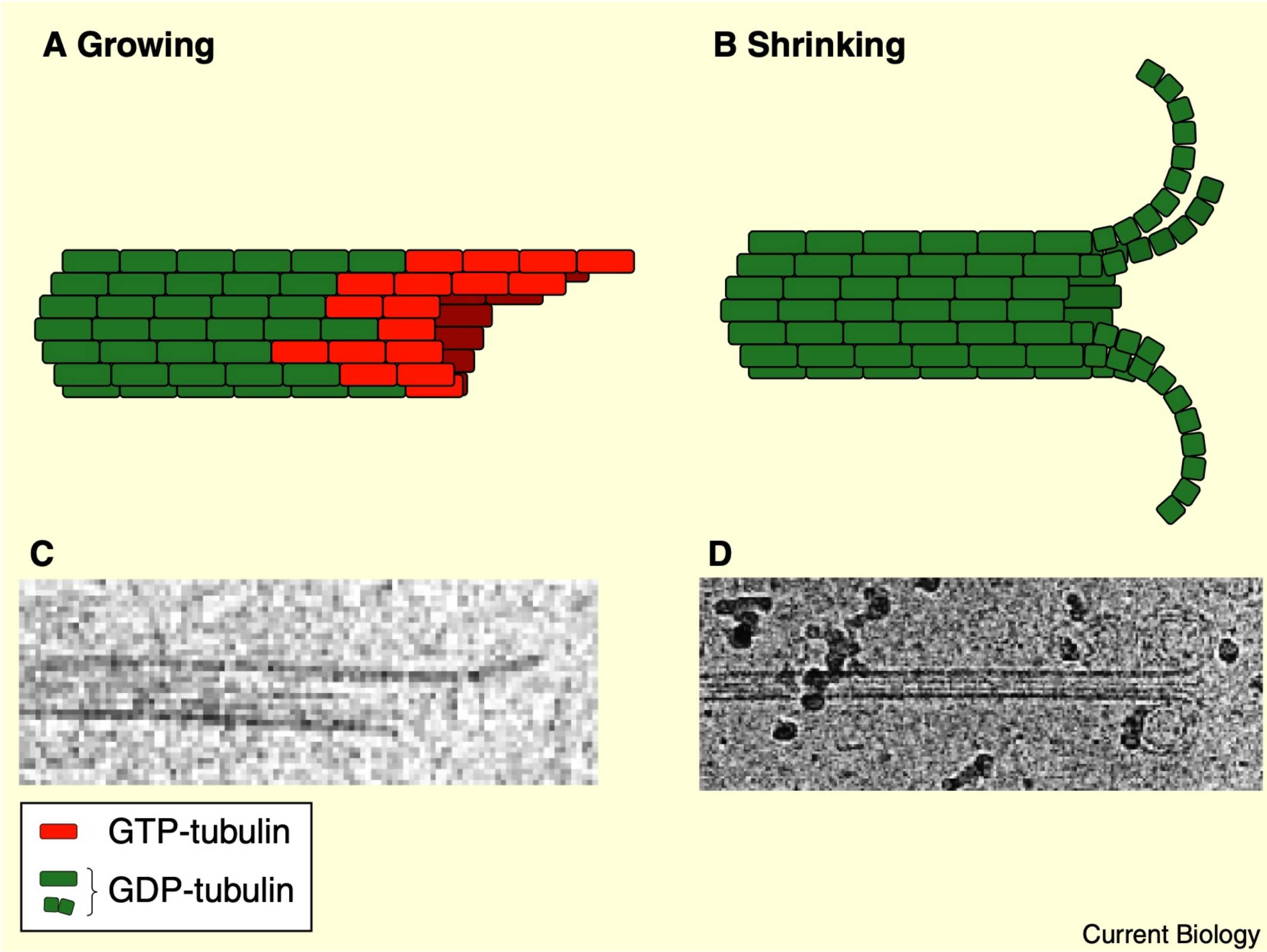


3. Treadmilling

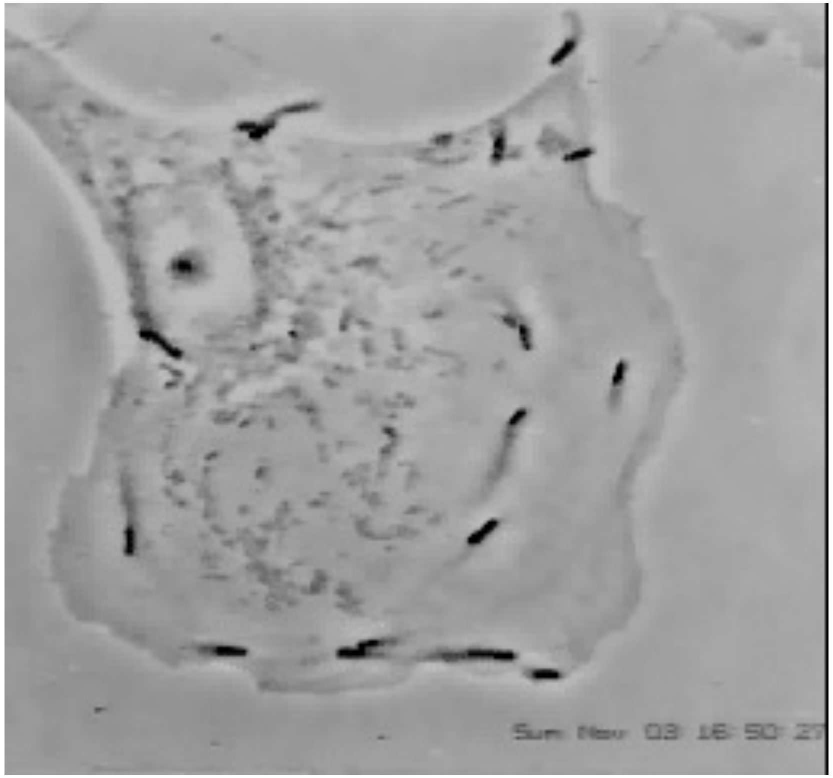


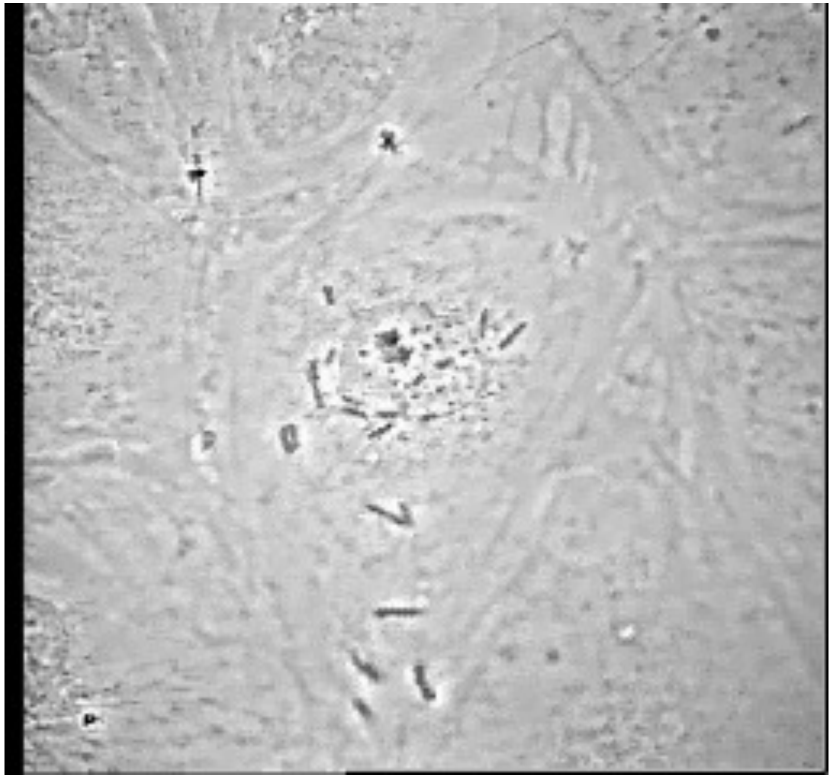


Dynamic instability



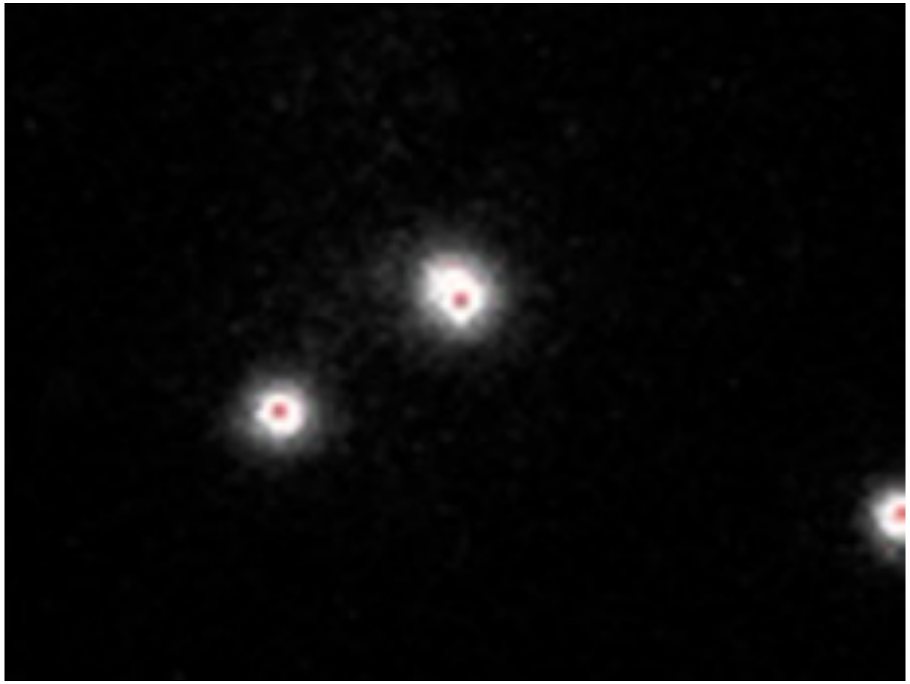
Motility with polymerization





Motility with polymerization *In Vitro*

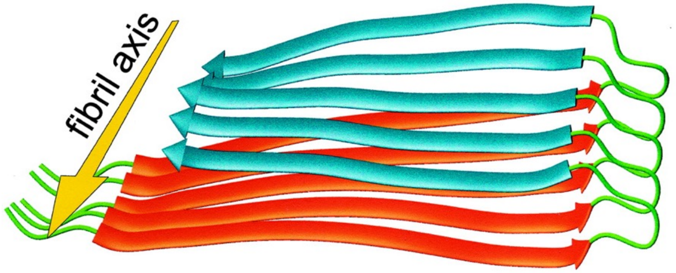
Microbeads coated asymmetrically with ActA, in Xenopus extract

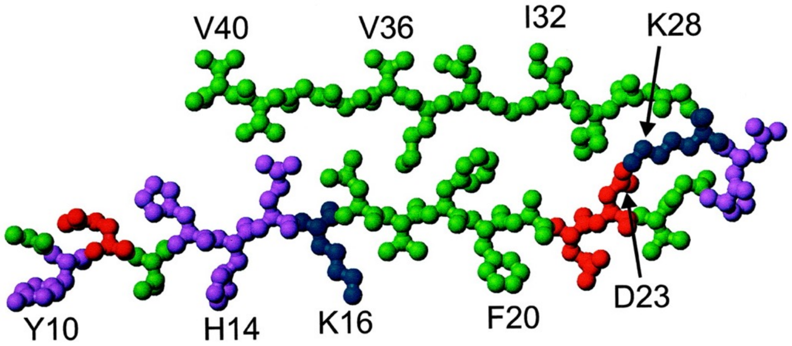


Microbeads coated symmetrically with ActA, in Xenopus extract

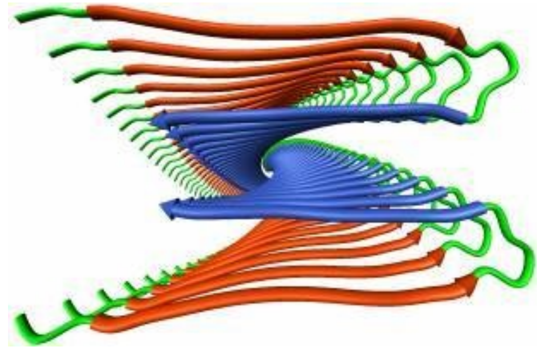
Self assembly, guided polymerization

Amiloid ß-fibrils: Alzheimer plaques

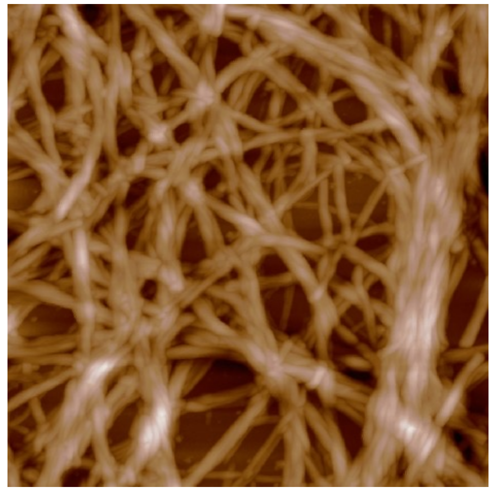




Amyloid ß1-40 peptide

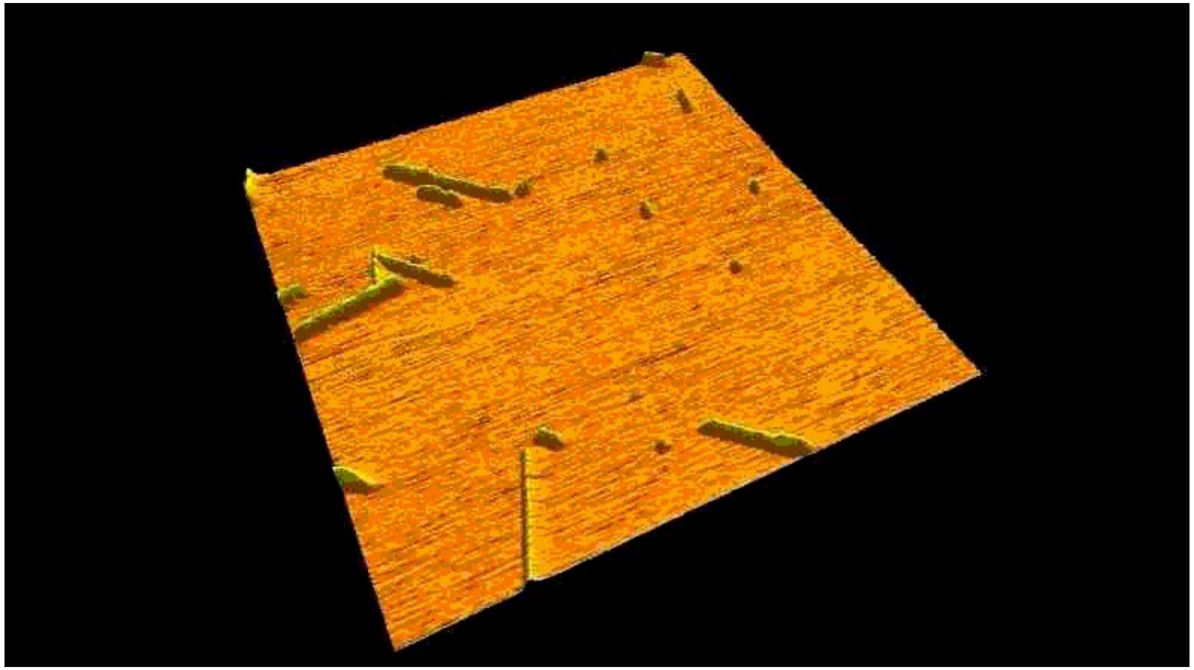


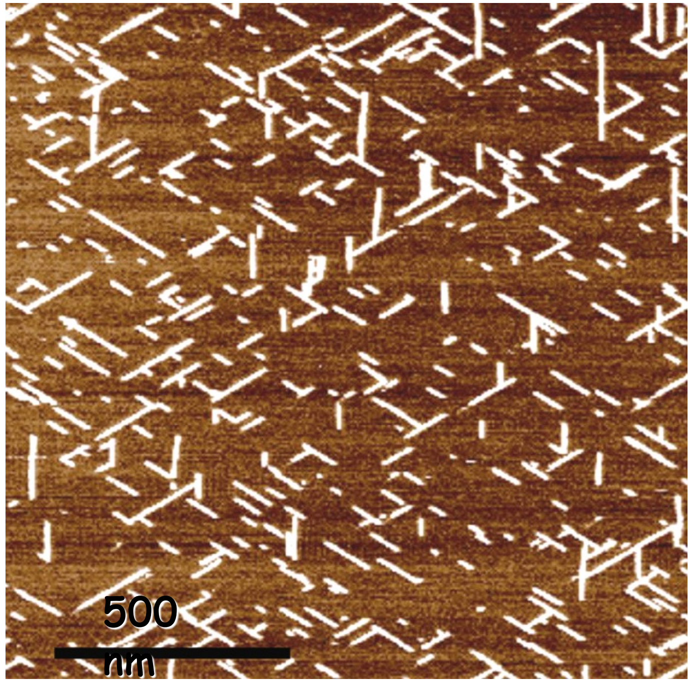
Aß1-40 protofilament



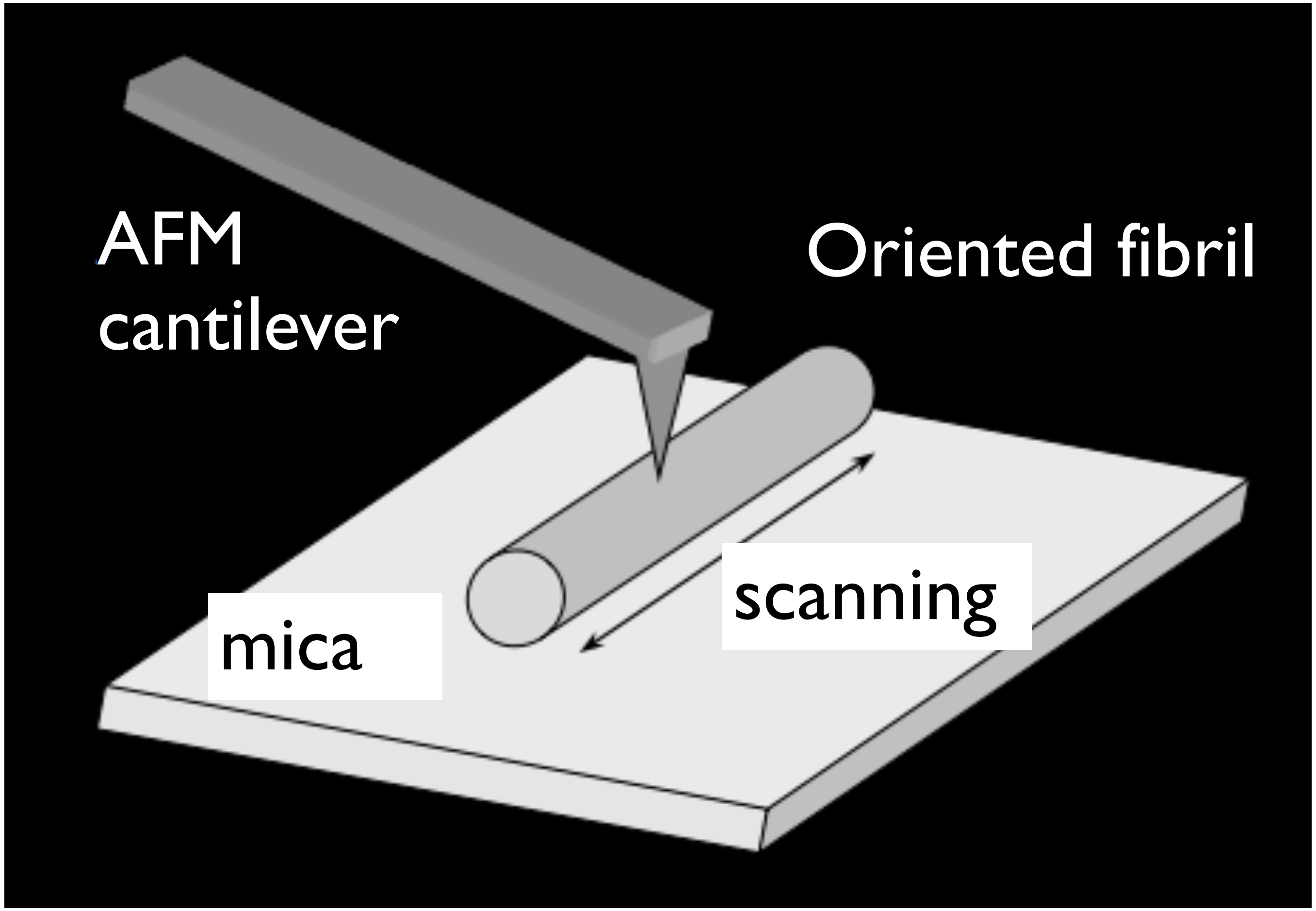
in vitro grown fibrills (AFM)

Epitaxial growth of amyloid fibrils on mica surface





Growth of amyloid fibrils studied by AFM



Spatial resolution: 1 nm

Temporal resolution: 300 ms

Kymography of amyloid growth