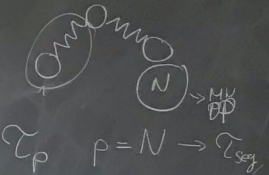


Macromolecular Dynamics

Rouse Model


 τ_p $p=N \rightarrow \tau_{seg}$

$$\zeta = 6\pi\eta_s a$$

$$\tau = \frac{dG(\text{free enthalpy})}{dx} = -T \frac{d}{dx} \ln P$$

$$= -kT \left[\frac{d}{dx} \left(\text{const} - \frac{3}{2b^2} x^2 \right) \right] = \left(\frac{3kT}{b^2} \right) x$$

$$D = \frac{kT}{\zeta} \quad \tau \sim \frac{R^2}{D} = \frac{R^2 \left(\frac{p}{b} \right)}{kT}$$

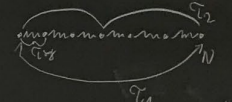
$$R_g = \frac{Nb}{\sqrt{6}} \quad (\theta\text{-conditions})$$

$$\tau_p = \left(\frac{N}{p} \right)^2 \tau_{seg} \quad \tau_{seg} \sim \frac{b^2 \zeta}{kT}$$

$$\tau_{Rouse} \sim \frac{\zeta b^3}{kT} (N^2)$$

$$\tau_1 \sim M^2 \quad [\eta] \sim M$$

$$D_t \sim M^{-1}$$


 τ_1 τ_2

$$G^{\perp} = G^{\perp} + iG^{\parallel}$$


Rouse Model

$$G' = \frac{cRT}{M} \sum_{p=1}^N \frac{(\omega \tau_p)^2}{1 + (\omega \tau_p)^2}$$

$$G'' = \omega \eta_s + \frac{cRT}{M} \sum_{p=1}^N \frac{\omega \tau_p}{1 + (\omega \tau_p)^2}$$

$$[G'] \equiv \lim_{c \rightarrow 0} \left(\frac{G'}{c} \right)$$

$$[G'] = \lim_{c \rightarrow 0} \left(\frac{G'' - \omega \eta_s}{c} \right)$$

$$[G']_{\text{Rouse}} = \frac{M}{RT} [G']$$

$$[G'']_R = \frac{M}{RT} [G'']$$

$$G(t) \sim \frac{\hbar T}{b^3} \gamma \left(\frac{t}{\tau_{\text{seg}}} \right)^{-1/2} \exp \left(-\frac{t}{\tau_R} \right)$$

Rouse

$$\tau_R \approx \frac{\eta_s b^3 N^2}{\hbar T}$$

$t < \tau_{\text{seg}}$ does not move

$t > \tau_R$ diffusion = liquid

$\tau_{\text{seg}} < t < \tau_R$ Viscoelastic behavior

$\tau_{\text{rep}} \sim \frac{L^2}{D} \sim N^3$
 $D \sim \frac{R^2}{\tau_{\text{rep}}} \sim N^{-2}$

$\tau_{\text{Darcy}} \sim N^2$
 $\tau_{\text{Zimm}} \sim N^{3/2}$

De Gennes reptation model