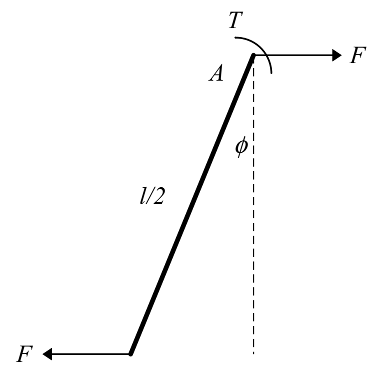
Prob 2. 19

`Estimate for the theoretical stiffness of a polymer molecule.`

Consider half of a polymer link:



The force along the link direction is $F_l = F \sin\theta$, and the torque around point *A* is $T = F\,(l/2)\cos\phi$. The strain energy is then

$$U = n\left[U_l + U_\phi\right] = n\left[\frac{F_l^2}{2k_l} + \frac{T_\phi^2}{2k_\phi}\right]$$

$$= n\left[\frac{(F\sin\phi)^2}{2k_l} + \frac{\left(F\frac{l}{2}\cos\phi\right)^2}{2k_\phi}\right]$$

Castigliano's Theorem then gives the deflection as

$$\delta = \frac{\partial U}{\partial F} = n\left[\frac{2F\sin^2\phi}{2k_l} + \frac{2F\left(\frac{l}{2}\cos\phi\right)^2}{2k_\phi}\right]$$

$$= nF\left[\frac{\sin^2\phi}{k_l} + \frac{l^2\cos^2\phi}{4k_\phi}\right]$$

The effective spring stiffness *k* from $F = k\,\delta$ is then

k[eff]:= (n*(sin(phi)^2/(k[l]) + l^2*(cos(phi)^2/(4*k[phi]))))^(-1);

$$k_{eff} := \frac{1}{n\left(\frac{\sin(\phi)^2}{k_l} + \frac{1}{4}\frac{l^2\cos(\phi)^2}{k_\phi}\right)}$$

T modulus is then $E = k_{eff}L/A$. The extended chain length is $L = nl\sin\phi$ and the effective chain area from crystallographic measurements is 0.181 nm^2:

L:=n*l*sin(phi); l:=153e-12;phi:=(56*Pi/180);A:=.181e-18;

k[l]:=435;k[phi]:=35;

The modulus (in Pa) is then:

Digits:=4;'E'=evalf(k[eff]*L/A);

$$E = .4435\ 10^{12}$$

This is more than twice the stiffness of steel, at a fraction of the weight.