Electronic Supplementary Material (ESI) for Soft Matter

Electronic Supplementary Information (ESI)

Force field parameters

The total bond energy is the sum of four contributions:

$$U_{bond} = U_l + U_\phi + U_\theta + U_\lambda,$$

with:

$$\begin{aligned} U_l &= \frac{k_l}{2}(l-l_0)^2 \\ U_\phi &= \frac{k_\phi}{2}(\phi-\phi_0)^2 \\ U_\theta &= 1 + a_2\theta^2 + \theta^4 + a_6\theta^6 \\ U_\lambda &= \frac{k_\lambda}{2}(|\lambda|-\lambda_0)^2 \end{aligned}$$

where l and ϕ denote bond length and bond angle, respectively. Dihedral angles (see Fig. 1a in the main text) are denoted by λ and θ. The parameters of the force field parameters are given in Table 1. The values of a_2 and a_6 were computed for each θ_0 to get the potential with minima at $\pm\theta_0$ and a barrier height of $\Delta E = 5/2$.

term	beads affected	parameters
$U_{l_{BS}}$	$B-S$	$k_l = 50$, $l_0 = 2$
$U_{l_{BS}}$	$B-B$	$k_l = 100$, $l_0 = 1$
$U_{\phi_{SBB}}$	$S-B-B$	$k_\phi = 200$, $\phi_0 = 90°$
$U_{\phi_{BBB}}$	$B-B-B$	$k_\phi = 50$, $\phi_0 = 180°$
U_λ	$S-B_iB_{i+2}-S$	$k_\lambda = 10$
U_θ	$S1-B_iB_{i+1}-S2$	a_2 and a_6 - see the text
LJ	B	$\varepsilon = 1$, $\sigma_B = 4$
LJ	$S1, S2$	$\varepsilon = 1$, $\sigma_S = 1$

Table 1 Force field parameters

Simulations

Simulations were run with the LAMMPS package in three stages:

1. Short equilibration of side strands with backbone beads' location restrained: timestep=$0.5\times10^{-3}t_D$, total time=$40t_D$
2. Short molecular dynamics NVT run at $T^* = 1.5$ in order to relax the initial configuration run to change the initial configuration of the fibrils: timestep=$10^{-2}t_D$, total time=$800t_D$
3. Langevin dynamics: timestep=$10^{-2}t_D$, total time=$10^6 t_D$

Helix angle

As illustrated in Fig. 1, the helix angle, α_0 is the angle between the helical curve and the vertical axis. The arc a is spanned by horizontal vectors ρ_1 and ρ_2 with λ_0 being the angle between them. Next, b is the axial distance between the two consecutive side strand beads. The length of arc a is therefore $\rho\lambda_0$, where $\rho = |\rho_1| = |\rho_2|$ is the radius of the cylinder containing the helix. The lines a (dashed), b (dotted), and s (segment of a helix) form a right triangle, hence $\tan(\alpha_0) = \frac{\rho\lambda_0}{b}$. In our case ρ corresponds to $l_{BS} = 2$, whereas b is $b = 2l_{BB} = 2$. Hence, $\tan(\alpha_0) = \lambda_0$ and $\alpha_0 = \arctan(\lambda_0)$.

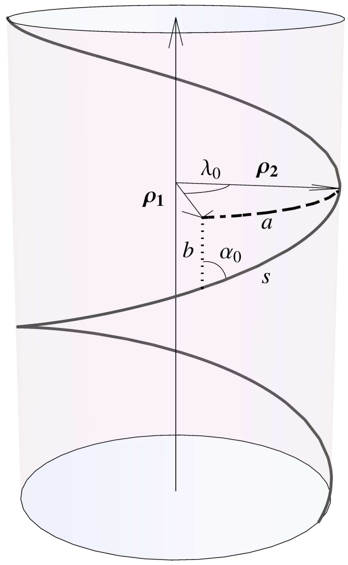

Fig. 1 Schematic illustrating the relation between the angles α_0 and λ_0.

Relation of the chirality, χ, to the torsion of the chain

Below we show that in the limit of a continuous curve Eq. (2) gives the local torsion of the chain. Consider a curve parametrized by its arc length, s. and three consecutive tangent vectors $\mathbf{t}_- = \mathbf{t}(-\varepsilon)$, $\mathbf{t} = \mathbf{t}(0)$ and $\mathbf{t}_+ = \mathbf{t}(\varepsilon)$, separated by a distance ε along the arc length. The tangent vectors, together with the corresponding normal and binormal vectors constitute a local orthogonal trihedron fulfilling the Frenet-Serret relations

$$\mathbf{t}' = \kappa \mathbf{n}$$

$$\mathbf{n}' = -\kappa \mathbf{t} + \tau \mathbf{b}$$

$$\mathbf{b}' = -\kappa \mathbf{t}$$

where κ is the curvature and τ is the torsion of the curve. The prime denotes differentiation with respect to the arc length. For small ε

$$\mathbf{t}_\pm = \mathbf{t} \pm \mathbf{t}'\varepsilon + \frac{1}{2}\varepsilon^2 \mathbf{t}'' + \dots$$

Using Frenet-Serret formulas

$$\mathbf{t}_\pm = \mathbf{t} \pm \kappa \mathbf{n}\varepsilon + \frac{1}{2}\varepsilon^2(\kappa' \mathbf{n} - \kappa^2 \mathbf{t} + \kappa\tau \mathbf{b}) + O(\varepsilon^3)$$

which leads to

$$\mathbf{t}_- \times \mathbf{t} = \kappa\varepsilon \mathbf{b} + \frac{1}{2}\varepsilon^2(\kappa\tau \mathbf{n} - \kappa' \mathbf{b})$$

and

$$\mathbf{t} \times \mathbf{t}_+ = \kappa\varepsilon \mathbf{b} - \frac{1}{2}\varepsilon^2(\kappa\tau \mathbf{n} - \kappa' \mathbf{b})$$

Finally

$$(\mathbf{t}_- \times \mathbf{t}) \cdot (\mathbf{t} \times \mathbf{t}_+) = \kappa^2 \varepsilon^2 + \dots$$

and

$$(\mathbf{t}_- \times \mathbf{t}) \cdot \mathbf{t}_+ = \kappa^2 \tau \varepsilon^3 + \dots$$

The argument of the arc tangent function in Eq. (2) is the ratio of these two terms. Thus, in the limit of small ε the expression $\text{arctan2}\Big(|\mathbf{v}_i|\mathbf{v}_{i-1} \cdot (\mathbf{v}_i \times \mathbf{v}_{i+1}),\ (\mathbf{v}_{i-1} \times \mathbf{v}_i) \cdot (\mathbf{v}_i \times \mathbf{v}_{i+1})\Big)$ is proportional to the local (signed) torsion of the chain.