

# Treating d-banding as a phase field

I would like to couple d-banding of fibrils into the current free energy picture of the system. One way to do this is to use a phase-field-crystal model approach [?], in which the periodic density modulations are described by an additional term in the free energy functional. To start with, I consider the free energy functional  $F$  of a cylinder with a radius  $R$ , length  $L$ , and some internal structure given by a director field  $\mathbf{n}(\mathbf{r})$  and a density  $\rho(\mathbf{r})$ , which is surrounded by a fluid. I'll suppose that the surface tension  $\gamma$  between the cylinder and the fluid depends on whether it is measured on the cylinder's side (with area  $2\pi RL$  and  $\gamma = \gamma_s$ ), or on one of the two cylindrical caps (each with area  $\pi R^2$  and  $\gamma = \gamma_t$ ). The total free energy is then

$$F(R, L) = \int_0^R \int_0^L \int_0^{2\pi} f(\mathbf{r}, \mathbf{n}(\mathbf{r}), \rho(\mathbf{r})) r dr dz d\phi + 2\pi RL\gamma_s + 2\pi R^2\gamma_t. \quad (1)$$

The equilibrium configuration is determined by minimization of eqn 1 with respect to  $R$ ,  $L$ ,  $\mathbf{n}(\mathbf{r})$ , and  $\rho(\mathbf{r})$ .

To make this problem tractable, there are several assumptions that must I'm going to apply. The first assumption is that the director field follows a double-twist, so  $\mathbf{n}$  is reduced to a single twist field  $\psi(r)$  which is dependent only on the radius. With no consideration of density fluctuations, this reduces the free energy  $f$  to the familiar Frank free energy of a double-twisted liquid crystal,

$$f_{dt} = -k_2 \left( \psi' + \frac{\sin 2\psi}{2r} \right) + \frac{1}{2} K_{22} \left( \psi' \frac{\sin 2\psi}{2r} \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4 \psi}{r^2} - \frac{1}{2} (K_{22} + k_{24}) \frac{1}{r} \frac{d \sin^2 \psi}{dr}. \quad (2)$$

The elastic constants  $k_i$  and  $K_j$  in eqn 2 are dependent on the density of the liquid crystal [?], and so density fluctuations may couple into the frank free energy. For this work, I will only allow for density fluctuations along the  $z$  axis of the cylinder to mimic the d-banding of fibrils. Without considering the coupling of density to eqn 2, an additional term from the phase-field-crystal literature can be introduced into the free energy of the form

$$f_{pfc} = \frac{b}{2} \rho(z) \left[ \lambda_0^2 + \frac{\partial^2}{\partial z^2} \right]^2 \rho(z). \quad (3)$$

Here,  $\lambda_0^{-1}$  is the length scale at which the d-banding occurs. For collagen fibrils, we make the

hypothesis that this length scale couples with the twist angle by the geometrical construction

$$\lambda_0 = \frac{2\pi}{d_0 \cos \psi(r)}, \quad (4)$$

where  $d_0 = 67 \text{ nm}$  is the d-band spacing for a fibril with no twist.

To build a tractable form of the free energy, I assume that the elastic constants are independent of the density variations, and assume  $\rho(z) = \rho_0 \cos(kz)$  (in the future, I may extend this to allow  $k$  to vary with  $r$  as well). Combining the two parts (eqns 2 and 3) into a single free energy, and setting  $q = 1$ ,  $K_{22} = 1$  (they scale out of the free energy anyway), the free energy per volume of fibril is

$$\begin{aligned} E &\equiv \frac{F}{\pi R^2 L} \\ &= \frac{2}{R^2} \int_0^R r dr \left[ -\psi' - \frac{\sin 2\psi(r)}{2r} + \frac{1}{2} \left( \psi' + \frac{\sin 2\psi(r)}{2r} \right)^2 + \frac{1}{2} K_{33} \frac{\sin^4 \psi(r)}{r^2} \right] - (1 + k_{24}) \frac{\sin^2 \psi(R)}{R^2} \\ &\quad + \frac{\Lambda}{2R^2} \left( 1 + \frac{\sin(2kL)}{2kL} \right) \int_0^R r dr \left( \left[ \frac{2\pi}{d_0 \cos \psi(r)} \right]^2 - k^2 \right)^2 + \frac{2\gamma_{\text{side}}}{R} + \frac{2\gamma_{\text{top}}}{L} \end{aligned} \quad (5)$$

Minimization of this free energy corresponds to a  $\psi(r)$ ,  $R$ ,  $L$ , and  $k$  which simultaneously satisfy the constraints

$$\frac{\delta E}{\delta \psi} = 0, \quad (6)$$

$$\frac{\partial E}{\partial R} = 0, \quad (7)$$

$$\frac{\partial E}{\partial L} = 0, \quad (8)$$

$$\frac{\partial E}{\partial k} = 0. \quad (9)$$

This is numerically difficult. My best idea so far is to use simulated annealing or gradient descent to determine  $R$ ,  $L$ , and  $k$ .

## References