Double twist liquid crystal model of collagen structure

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Collagen is the main component of connective tissue and the most abundant protein in mammals. The structure of collagen is hierarchical, with the triple-helical molecules organizing into fibrils, and fibrils contained in higher-order arrangements. A fibril may be considered as a liquid crystal of individual triple helices. Their chiral molecular structure can lead to a macroscopic helical arrangement known as the cholesteric phase, which has been observed in fragments of collagen fibrils. The cholesteric orientation can vary with radial distance in the fibril, this is known as a “double twist”. We numerically minimize the mean-field Frank free energy in the bulk to solve for the liquid crystal orientation as a function of radial distance, $\psi(r)$. By also considering surface terms, we find the optimal fibril radius R and molecule orientation on the fibril surface $\psi(R)$. We find that $K_3/K_2>>1$, where the twist modulus is much larger than the bend modulus, leads to a metastable minimum that recovers experimental measurements for R and $\psi(R)$ of collagen fibrils.