A LIQUID CRYSTAL MODEL FOR BILAYER LIPID MEMBRANES

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INTRODUCTION

Bilayer lipid membranes (BLMs) constitute the base component of cell membranes. They exhibit orientational order like crystal solids but they flow like amorphous liquids. Their rigidity permits confining the cell contents and preserving the cell shape while their ordered structure regulates the transport of substances in and out the cell. Their fluidity enables the transport phenomena to occur rather quickly. These peculiar properties are typical of liquid crystals. Indeed, BLMs are recognized to be Smectic liquid crystals since their molecules form layered structures with defined interlayer spacing. In particular, BLMs are classified as Smectic A liquid crystals due to the fact that their molecular axes are normal to the layers.

At CIMMS (Center for Intelligent Material Systems and Structures), preliminary experiments have been conducted to evaluate the maximum pressure that synthetic BLMs can withstand (Hopkinson et al., 2006). Together with experiments, constitutive models need to be developed not only to help the interpretation of the experimental results but also to guide the design of these experiments.

A mathematical model that describes the small deflections of a circular BLM under constant pressure will be presented. The model is formulated within the theoretical framework of the continuum theory of liquid crystals set forth by de Gennes (de Gennes and Prost, 1993).

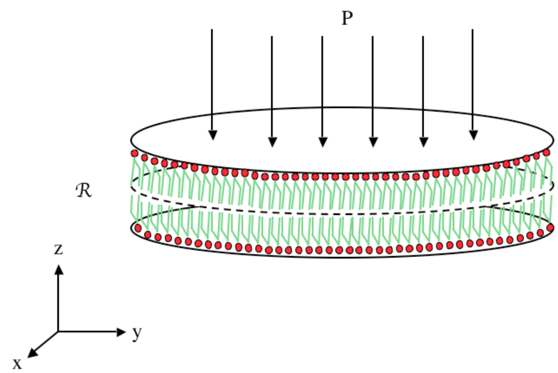

Figure 1: Coordinate system for the BLM.

MATHEMATICAL MODEL

Let R be the region occupied by the BLM and **n** a unit vector, called director, which defines the average alignment of the lipid molecules. Let consider a coordinate system as shown in Figure 1. If the BLM is assumed not to bend very much from the x-y plane and not to strongly compress, the bulk elastic energy has the form (de Gennes and Prost, 1993)

$$F = B\left(\frac{\partial u}{\partial z}\right)^2 + \frac{K_1}{2}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)^2 + \\ +2K_1\left(\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \frac{\partial^2 u}{\partial x^2}\frac{\partial^2 u}{\partial y^2}\right), \quad (1)$$

where $u(x,y,z)$ is the vertical displacement of the layer, B and K_1 are constants with energy length^{-3} and energy length^{-1} dimensions, respectively. The first term in equation (1) defines the compressive (dilatational) energy while the other terms define the elastic splay energy.

It is assumed that for small displacements to the initial alignment the director $\boldsymbol{n}$ is given by

$$\boldsymbol{n} \approx (-u_x,\ -u_y,\ 1),\ |u_x|,\ |u_y| << 1.$$

In the experimental study, the BLM is reconstituted over a polycarbonate substrate with cylindrical pores and, subsequently, subjected to hydrostatic pressure. For this reason, the energy integral that results from the sum of the bulk elastic energy and the work done by the constant pressure P per unit area acting on the BLM is considered. It has the form

$$\int_R B\left(\frac{\partial u}{\partial z}\right)^2 + \frac{K_1}{2}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)^2 + +2K_1\left(\left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 - \frac{\partial^2 u}{\partial x^2}\frac{\partial^2 u}{\partial y^2}\right) - Pu\ dR \quad (2)$$

The functional (2) need to be minimized to derive the equilibrium equations for the BLM by using variational methods

RESULTS AND DISCUSSION

The predictions of the model are obtained by assuming that the compression of the BLM is negligible and that the deflection of the circular BLM has radial symmetry. Under these assumptions, the solution of the equilibrium equations in polar coordinates with the origin in the center of the BLM is

$$u(r) = \frac{P}{64hK_1}\left(r^2 - R^2\right)^2, \quad (3)$$

where h is the thickness of the BLM and the edges of the circular BLM are considered to be clamped. In Figure 2, solution (3) is plotted for P=-1 kPa, R=0.4 μm, h=5 nm as dictated by preliminary experimental studies and for different values of elastic constant K_1.

Additional theoretical and computational studies are being performed to model the mechanical behavior of the BLMs under less restrictive assumptions on the form of the deflection. In addition, new experiments are being designed to accurately measure the pressure that the BLMs can withstand.

CONCLUSIONS

A continuum model that describes the small deflections of BLMs under constant pressure by accounting for their Smectic A liquid crystalline structure is proposed. The predictions of the model are obtained by assuming that the deflections have radial symmetry and by using values of the material parameters that are suggested by preliminary experimental observations.

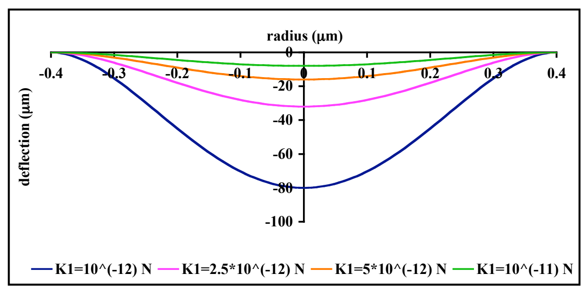

Figure 1: Deflection u of a circular BLM plate of radius r under constant pressure.

REFERENCES

de Gennes, P.G., Prost, J.Y. (1993). *The Physics of Liquid Crystals,* Oxford Science Publications, second edition.

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