A Continuum Model to describe the Elastic Behavior of Multilamellar Lipid Bilayer Membrane using Molecular Dynamic Simulation

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Abstract

Lipid bilayer membranes are ubiquitous to biological systems and have been extensively studied for their ability to form non-covalent barriers between two fluid mediums (e.g. cell membrane). In synovial joints (knee, hip etc), multilamellar membranes, which consist of a stack of phospholipid bilayer membranes separated by layers of water molecules, have been identified to coat cartilaginous surfaces. It is hypothesized that multilamellar membranes play an essential role in the lubrication of synovial joints. Synovial joints in the body allow for a range of motion between two articulating surfaces. While functioning optimally, i.e. without disease or injury, these joints exhibit very low friction and no wear characteristics. Furthermore synovial joints maintain a constant lubrication regime in the joint cavity, i.e. it does not drain under gravity and perhaps most remarkably resists anisotropic compression applied during normal joint function. Our hypothesis speculates that phospholipids, in particular are responsible for resisting anisotropic compression in the joint, governed by the elastic behavior of multilamellar membranes. The focus of this work is the fundamental study of the mechanical response of an elastically stretched lipid bilayer membrane as a function of hydration, or concentration of water per phospholipid. One expects that the elastic modulus, K_A is governed by complex phenomena related to atomistic interactions between phospholipid/phospholipid and phospholipid/water. Therefore in order to elucidate these phenomena, a series of molecular dynamic simulations of a model DPPC bilayer, (as defined in Marrink *et al.*, 2007) with various levels of hydration and compression were performed. The bilayer was subjected to a compressive force normal to the bilayer surface while the directions parallel to the bilayer are maintained at atmospheric pressure. The discussion is driven by our goal to derive a continuum model to describe the elastic behavior of multilamellar lipid membranes.

References

Marrink, S.J., Risselada, H.J., Yefimov, S., Tieleman, D.P. & de Vries, A.H. 2007 The MARTINI forcefield: coarse grained model for biomolecular simulations. *J. Phys. Chem. B* **111** (27), 7812–7824.