MOLECULAR DYNAMICS OF MODEL MEMBRANES

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We have applied the method of molecular dynamics (M.D.) to a model of a biological membrane. The M.D.method is essentially a procedure for numerical integration of Newton's equations of motion for a large number of particles on the basis of a known interaction potential. Our model consists of two layers of 16 decanoate molecules each and is periodic in two dimensions. Full simulations involving bond length constraints only were carried out over periods of 80 ps. The aim of this research is to get an understanding of the macroscopic properties of the system in terms of molecular interactions.

Of the various statistical analysis made on the computational results, we present the following features:
a. Calculated order parameters S_{CD} (defined as $\langle\frac{1}{2}(3\cos^2\theta - 1)\rangle$, where θ is the angle between the CD bond direction of deuterated decanoate and the bilayer normal) are in excellent agreement with measured values. From the relation between different order parameters it follows that full rotational freedom around the molecular axis does not exist.
b. Considerable spatial correlations in the molecular orientation, showing a cooperative tilt, is observed over the entire unit cell. This cooperativity persists over tens of ps (fig.1).
c. The orientation of the molecular segmental planes appear to be strongly correlated with the plane in which the molecule is tilted (fig.3). The rotation of the molecule around the chain axis (φ) becomes more restricted with increasing tilt angle θ (fig.2).

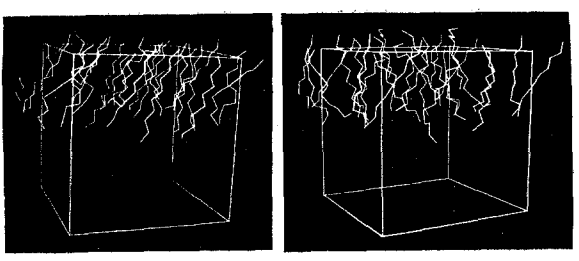

Fig.1. Two typical configurations taken from the simulation at a moment that a cooperative tilt of the molecules occurs (a) and at a moment when a more disordered structure prevails (b). For clarity only one half of the simulated bilayer is shown.

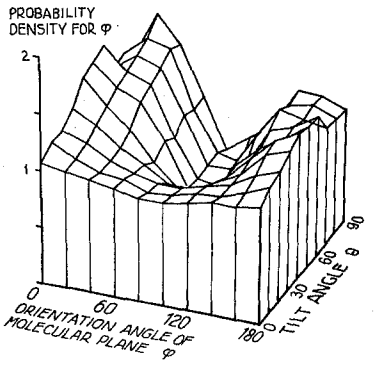

Fig.2. Distribution of the orientation angle φ of the molecular yz plane with respect to the plane in which the molecule is tilted (zN plane), as a function of the tilt angle θ. At large tilt angle there is a strong correlation: the molecule swings out as a knife blade in the direction in which it is thinnest.