Budapest University of Technology and Economics
Chemical Engineering Faculty, Department of Physical Chemistry

Structure determination of the model membranes with small angle scattering

PhD Theses

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Other Publications in English

VIII. T Drucker, A. Bóta: Description of the layer structure in centrosymmetric liposomes, Proceedings of the International School and Symposium on Small-Angle Scattering KFKI-1999-02/E (1999) 66.

IX. Bóta, T. Drucker, G. Goerigk, H.-G. Haubold: Layer formations in the pretransition range of DPPC/H_2O and DPPC/D_2O liposomes, DESY/HASYLAB Annual Reports (2000) 685.

X. T. Drucker, K. Szegedi, A. Bóta, G. Goerigk, S. Funari, Enhancing the diffraction data obtained with a 2D multiwire proportional counter DESY/HASYLAB Annual Reports (2003)

In Preparation

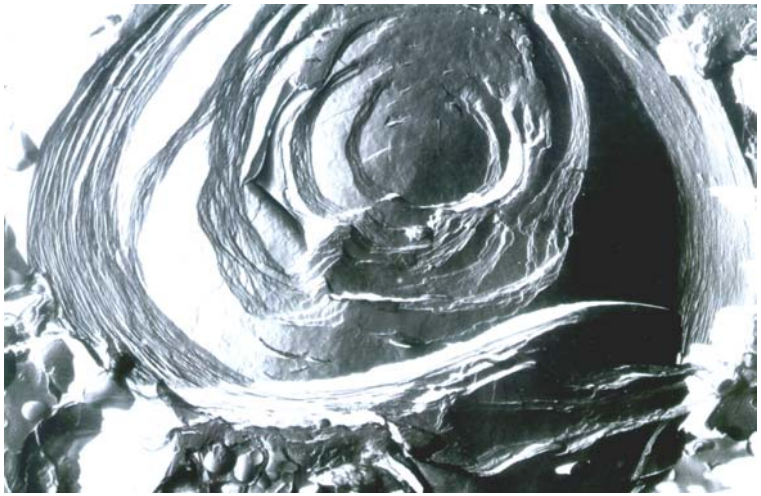
XI. T. Drucker, A. Bóta, Simulation of the small-angle X-ray scattering of liposomes, (2004)

Introduction

According to the old interpretation the phospholipid components of the biological membranes, in contrast to the membrane proteins, had only structural functions in the membrane mechanisms. This concept has been changed, because the liotropic liquid crystal of the nature of the phospholipid/water system might have influenced the membrane mechanisms.

I have chosen the 1,2-dipalmitoyl-phosphatidylcholine (DPPC)/water system as model membrane system, because the DPPC is one of the most common components in the biological membranes. The DPPC/water model system is a self-assembling system in which the phospholipid bilayers, and spherically symmetric shell-like multilamellar aggregates, liposomes are formed spontaneously. The system exhibits four liotropic liquid crystal phases in the function of the temperature.

The typical repeat distance of the multilamellar structure is 60-70 Å, therefore the small angle scattering is an ideal method for the structure determination.



Freeze fracture electron micrograph of a DPPC/water liposome.

Publications related to the Theses

Publications in English

I. A. Bóta, T. Drucker, M. Kriechbaum; Zs. Pálfia; G. Réz: Layer formations of dipalmitoylphosphatidylcholine liposomes in the pretransition range, Langmuir 15 (1999) 3101.

II. T. Drucker, A. Bóta, S. Borbély: Layer Formations of DPPC Liposomes, Physica B 276 (2000) 503.

III. A. Bóta, G. Goerigk, T. Drucker, H-G. Haubold, J. Petró: Anomalous small angle X-ray scattering on a new, non pyrophoric Raney-type Ni-catalyst, Journal of Catalysis 205 (2002) 354.

IV. A. Bóta, T. Drucker, K. Szegedi, G. Goerigk, Heinz-Günter Haubold, T. Vad, Distribution of copper ions in fully hydrated DPPC/water vesicles as studied by anomalous small angle X-ray scattering, Biochim. Biophys. Acta (2004 elküldve)

Publications in Hungarian

V. A. Bóta, T Drucker, M. Kriechbaum: Liposomes as model membrane systems, Olaj, szappan, kozmetika 5 (1998) 244.

VI. A. Bóta, Á. Csiszár, T. Drucker, B. Horváth, S. Borbély, M. Kriechbaum, G. Réz, H.-G. Haubold, T. Vad: The structural properties of the Dipalmitoyl-lecitine/water liposomes, Magy. Kém. Foly. 106/12 (2000) 488.

VII. T. Drucker, A. Bóta: The simulation of the small angle X-ray scattering of liposomes with centrosymmetric model, Magy. Kém. Foly. 107/6 (2001) 234.

5) I have found that the ratios of the diffraction peak maxima are affected by the fluctuation of the layer thickness. [VII, XI]

6) I have observed a relation between the minimum value between adjacent Bragg reflections and the sign of the corresponding Fourier terms. [XI]

7) I have determined a relation among the full width at the half maximum, the number of the layers and the fluctuation of the layer thickness. At constant layer thickness the relation is equivalent to the Scherrer equation. [VII, XI]

8) I have developed a reconstruction-method for the determination of the average layer number existing in the multilamellar vesicles, the fluctuation of the layers, the distribution of the scattering length density and the distribution of the total scattering volume vs. number of layers. Using these results I have interpreted the behaviour of the gel, rippled gel and liquid crystalline phases of the dipalmitoylphosphatidylcholine/water liposome system. [XI]

Goal

It is a common goal of several disciplines, such as the biophysics of membranes, the physical chemistry of liquid crystals, and the physical chemistry of self assembling systems to determine the structural properties of model membranes, liposomes.

The current methods that are based on a qualitative approach, have validated the basic principles, therefore the emphasis is shifted towards a more quantitative approach. The main goal of my dissertation was to meet these needs, and to develop a method, which is capable of the precise structure determination of the liposome systems from the small angle scattering, and quantitative interpretation of the results.

Summary

During my PhD studies I worked on two topics: the interpretation of the small angle scattering of liposome systems, such as the DPPC/water system, and the development of the small angle scattering evaluation techniques.

In the interpretation of the small angle scattering I have developed a model, in which the fluctuation of the layer structure is considered. Then I studied the relation between the structural parameters of the centrosymmetric layer structure, and the properties of the small angle scattering curve.

The second topic was derived from the first, because I have found that the positional resolution of the detector, and the precision of the evaluation was worse than the precision required by the interpretation methods, at the Jusifa synchrotron beamline (DESY, Hamburg). Therefore I have changed the evaluation technique, so that the precision of the evaluation was

improved, and I have determined the torsion function of the detector, so that it can be considered in the interpretation.

Finally I have simulated the small angle X-ray scattering of the gel, rippled gel, and liquid crystal phases of the DPPC/water liposomes that were measured at the Jusifa beamline, and I have determined the structural properties of the system. Most of the known structural characteristics of the phases were reproduced in the simulation, and new properties, such as the fluctuation of the layer thickness, the number of layers in the liposomes were determined for the phases.

Theses

1) I have developed a new method for the determination of the centre of the centrosymmetrical, two-dimensional small angle X-ray scattering patterns that is based on the Descartes → polar coordinate transformation. The precision of the centre is several times better than the precision obtained by the method at the Jusifa beamline (Desy/Hasylab) [III, IV, X]

2) I have introduced a more precise radial averaging method. The method provides higher resolution scattering curves than the traditional method used at the Jusifa working station (Hamburg, Desy/Hasylab). [III, IV, X]

3) I have developed a method to determine the distortion function of the two-dimensional position sensitive detector. The distortion function and the resolution of the detector was obtained by using the small angle x-ray scattering of a reference sample (dipalmitoylphosphatidylcholine/water system). [X]

4) I have modelled the small angle X-ray scattering of spherical symmetric layer structures with the consideration of the defects of the layer arrangement. The radial scattering length density distribution was represented as terms of a Fourier series or as strip functions. The beginning of the radial electron distribution function and the thickness of the layers were considered as probability variables. [I, II, IV-IX, XI]