# Pressure dependence of the single membrane structure of DPPC aqueous solution

**Norifumi Yamada[1] (5514), Hideki Seto[2] (5403), Takayoshi Takeda[2] (5393), Hidekazu Nobutou[1] (5922), and Mika Ishioka[2] (8364)**

[1]Graduate School of Bio-Sphere Science and [2]Faculty of Integrated Arts and Sciences , Hiroshima University, Higashi-Hiroshima 739-8521, Japan.

In excess water, dipalmitoyl-phosphatidylcholine(DPPC) self-assembles into multilamellar vesicles consisting of bilayers which display various structures with changing conditions. It is believed that pressure induces the interdigitated gel phase in which the structure of lipid membrane is much different from other phases.[1] However, there is no evidence that the membrane structure at pressure-induced phase is really interdigitated. In order to clarify this point, we performed small angle X-ray scattering (SAXS) experiments at BL40B2.

Incident X-ray beam was monochromatized to be 1Å and the sample-detector distance was 1m. A high-pressure cell developed for SAXS[2] was used and the measurement was done at 30≤T≤50°C and 0.1≤P≤120MPa. As a sample, 5wt.% of DPPC was dissolved in a saline with 7mM of $CaCl_2$ in order to expand a distance between bilayers over 300Å.[3] Thus, an inter-bilayer structure factor could be unity and only a single membrane scattering should be considered in the data analysis. Typical SAXS profile is shown in Fig.1 and no bragg peak from the lamellar structure was observed. The scattering intensity $I(q)$ is discribed by the following equation.

$$I(q) = |F(q)|^2/q^2 + I_{diff},$$

where $F(q)$ is the form factor of the lipid bilayers and $I_{diff}$ is the diffuse scattering due to density fluctuations of lipid molecules. We calculated $F(q)$ with the model given by Pabst[4] and $I_{diff}$ with the model by Nallet[5]. The result of fitting is shown by the solid line in Fig.1. The obtained parameters were consistent with the values in literature.[6]

Figure2 shows pressure dependence of the obtained parameters at 50°C. The drastic change at 40-45MPa is due to the phase transition from the liquid crystalline phase to the ripple gel phase. This transition pressure is consistent with the result of light transmittance experiment.[1] However, no change was observed around 100MPa where we expected the transition pressure to the interdigitated gel phase.

**Reference**

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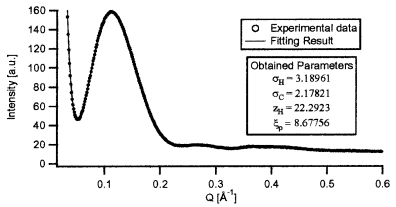


FIGURE 1. SAXS profile obserbed at 30°C and 0.1MPa.

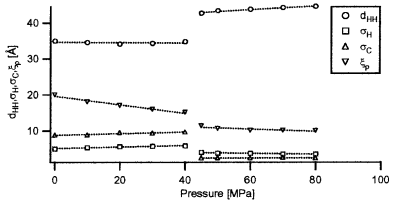


FIGURE 2. Pressure depencence of the fit parameters at 50°C; the head to head distance in the bilayer $d_{HH}$, standard deviation of electron density of the bilayers in the part of head $\sigma_H$ and the end of tail $\sigma_C$, and correlation length of concentration fluctuation $\xi_\rho$.



# Application of Small Angle X-ray Scattering for Expectation of Structures of Protein Molecules

**Katsuaki INOUE (1222), Toshihiko OKA (1327) and Naoto YAGI (1129)**
Life & Environment Division, Spring-8, JASRI, Mikazuki, Sayo, Hyogo 679-5198 JAPAN

BL40B2 is for recording small-angle x-ray scattering from non-crystalline biological materials. The light source is a bending magnet and the white x-rays generated by the bending magnet are monochromatized using a double crystal monochromator and focused by a 1-m-long rhodium coated cylinder mirror. The flux, when the ring current was 100 mA, is estimated to be $1 \times 10^{11}$ photons/sec at 1 Å (At the other wavelength, the flux is in same order). In this condition, the energy resolution (δE/E) is in the order of $10^{-4}$. The beam size is 250 μm (horizontal)×200 μm (vertical) (FWHM) at the detector position. The tunable energy range is 0.7 Å ~ 1.8 Å. Four sets of quadrant slit are set in the experimental hutch. For correcting the beam shape and removing the parasitic scattering, one or two sets of slit will be used. Two fixed-length vacuum paths allow camera lengths of 400 mm and 1000 mm. As a detector, an imaging plate area detector (RIGAKU R-AXIS IV++) is installed. This beamline was designed to be suitable for static measurements with high accuracy and high resolution. However, so far, this optics was not good for the SAXS measurements because the smallest q-range that could reach with such optics was not so small.

So, in order to get the scattering data with high small angle resolution, we tried to improve the optics set up, before performing the small angle scattering experiments for many kinds of protein solutions. As a results, the collimator whose diameter is about 1.2 mm is very effective to remove the parasitic scattering and it was clear that the minimum q-range of 0.007 Å$^{-1}$ can be achievable. In the case that the wavelength is 1.5 Å and the camera length is 1 m, the measurable q-range is estimated to be 0.007 ~ 0.6 Å$^{-1}$ (900 ~ 10 Å in Bragg spacing). In the case that the wavelength is 0.7 Å and the camera length is 400 mm, the measurable q-range can get longer up to 3.2 Å$^{-1}$ (1.9 Å in Bragg spacing ). This indicates that the optics and the measurement set up of BL40B2 are suitable for the static experiments.

In the next period, we will practically measure the scattering of some kinds of proteins.