



	<b>Experiment title:</b> The influence of oxidized phospholipids on vertical fine structures and electrostatics of phospholipid membranes	<b>Experiment number:</b> SC-3704
<b>Beamline:</b> ID10B	<b>Date of experiment:</b> from: 19.06.2013 to: 25.06.2013	<b>Date of report:</b> 02.08.2013
<b>Shifts:</b> 18	<b>Local contact(s):</b> Dr. Oleg Konovalov	<i>Received at ESRF:</i>

**Names and affiliations of applicants** (\* indicates experimentalists):

- A. Korytowski\* (Univ. Heidelberg)
- Dr. F. Rossetti\* (Univ. Heidelberg; iCeMS, Kyoto)
- A. Körner\* (Univ. Heidelberg)
- Dr. A. Makky \* (Univ. Heidelberg)
- A. Yamamoto\* (iCeMS, Kyoto)
- Dr. S. Inoue\* (Univ. Heidelberg; Kao, Corporation, Wakayama)
- Prof. Dr. M. Tanaka (Univ. Heidelberg)

**Report:**

The main goal of this experiment was to resolve the fine structures and electrostatics of phospholipid membranes in the presence and absence of oxidized phospholipids on different buffers to discriminate the interactions of different ions with the membrane.

Therefore, we simultaneously measured GISAXS/GIXF of phospholipid monolayers at the air/water interface in using the Langmuir film balance setup available at ID10. As a matrix phospholipid, we used OPPC and incorporated each of two oxidized phospholipids (OxPI) in a molar ratio of 10%, bearing either carboxyl or aldehyde group (PazePC and PoxnoPC).

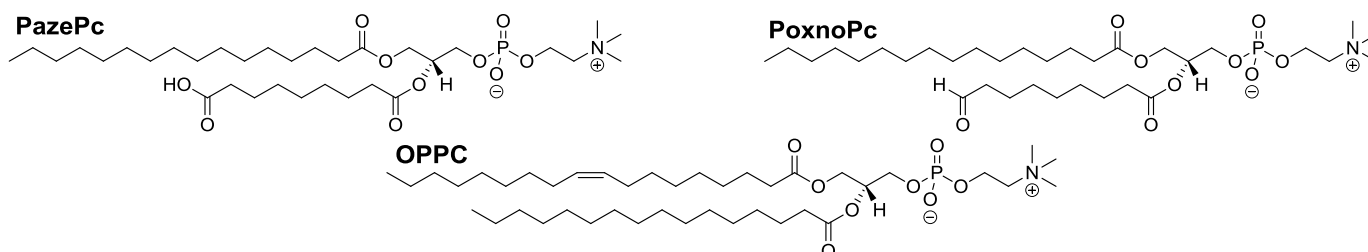


Figure1: Oxidized phospholipids studied in this experiment: (left) 1-palmitoyl-2-azelaoyl-sn-glycero-3-phosphocholine (**PazePC**), and (right) 1-palmitoyl-2-(9'-oxo-nonanoyl)-sn-glycero-3-phosphocholine (**PoxnoPC**). Both OxPI were mixed with the matrix lipid (bottom) 1-(9Z-octadecenoyl)-2-hexadecanoyl-sn-glycero-3-phosphocholine (**OPPC**).

Thus, the systems studied were: (a) **pure OPPC**, (b) **PazePC/OPPC (0.1)**, (c) **PoxnoPC/OPPC (0.1)** (d) **pure PazePC** and (e) **pure PoxnoPC**. Then these mixtures were spread onto (i) KCl, (ii) CaCl<sub>2</sub> and (iii) CsCl buffers at fixed surface pressure (20 mN/m) to

determine the membrane fine structures perpendicular to the interface and the location (concentration profile) and quantity of monovalent ( $K^+$ ,  $Cs^+$ ,  $Cl^-$ ) and divalent ( $Ca^{2+}$ ) ions near the interface.

Due to the high brilliance of the synchrotron beam we could clarify a different molecular structure of the different phospholipid membranes and determine a complete different behavior near the interface, especially for the divalent ion  $Ca^{2+}$ . Figure 2 represents the recorded GISAXS measurement for the system PazePC/OPPC and its electron density profile perpendicular to the membrane.

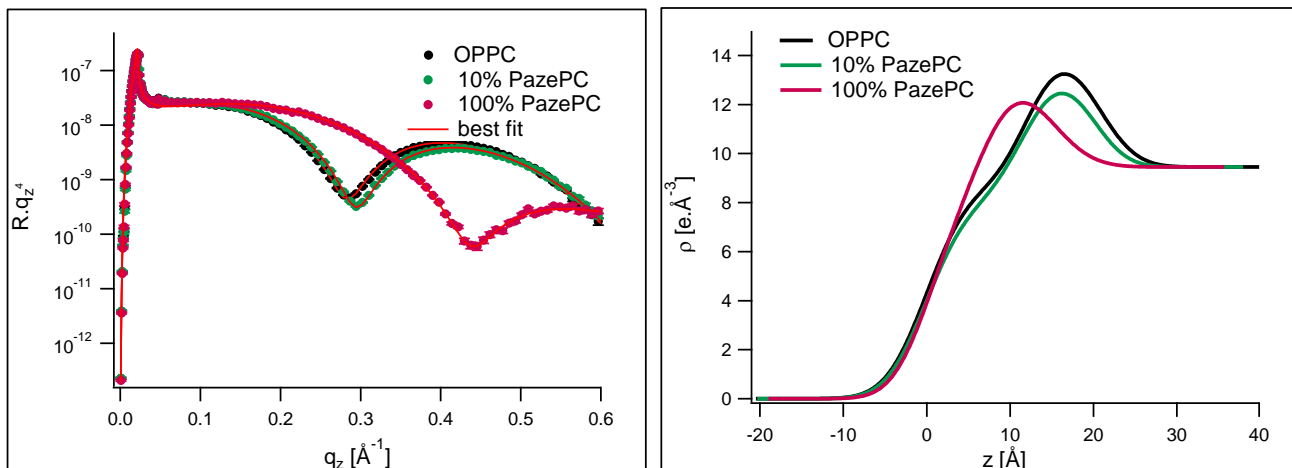


Figure 2: GISAXS measurement for the system PazePC/OPPC and its electron density profile perpendicular to the membrane.

Especially the sensitiv GIXF measurements of these systems show unique results for the ion concentration profiles and enables us to calculate the number of ions near the interface (Figure 3).

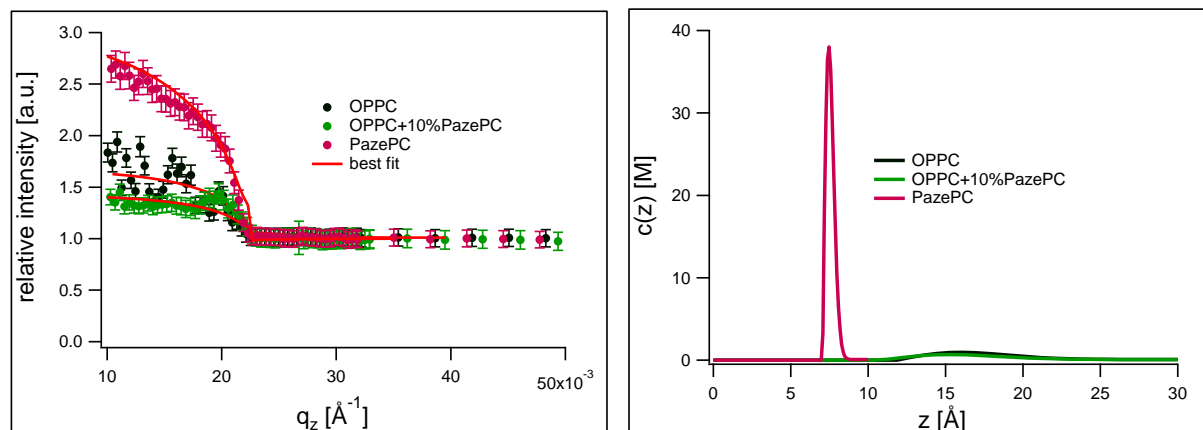


Figure 3: GIXF measurement for the system PazePC/OPPC and the concentration profile of  $Ca^{2+}$  near the air-water interface.

These experimental findings can be now combined with our results from surface pressure and surface potential measurements (performed at Univ. Heidelberg). Because this project is an interdisciplinary challenge, we will compare our gained experimental results with theoretical modeling (Prof. P. Jungwirth, Prague) to provide our understanding of the impact of oxidized phospholipids on a molecular basis to the scientific community.