ARTICLE TYPE

Supplementary Information: The Picosecond Dynamics of the Phospholipid Dimyristoylphosphatidylcholine in Mono- and Bilayers

Sebastian Busch,*a Luis Carlos Pardo,^b Christoph Smuda,^c and Tobias Unruh*a,d

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1 Thin Layer Chromatography

Thin layer chromatography (TLC) was performed on aluminium sheets covered with HPTLC Silica gel 60 F_{254} (Merck KGA, Darmstadt, Germany). Two measurements with different eluents were performed:

- 1. cyclohexane/isopropanol/water 30/40/6 (V/V), the procedure described in application #400710 of Macherey-Nagel, and in the literature¹.
- 2. chloroform/methanol/water 65/25/4 (V/V), described by Avanti Polar Lipids, Al, USA.

An UV lamp was used to make the substances visible.

2 Differential Scanning Calorimetry

Differential scanning calorimetry (DSC) was performed on a Setaram microDSC. 0.1 ml of sample (DMPC multibilayers in H_2O and DMPC multibilayers in D_2O) were measured against 0.1 ml of H_2O or D_2O , respectively, with a cooling/heating rate of 0.1 K/min. The shifts of the phase transition temperatures induced by the H_2O/D_2O exchange is only minor as can be seen in figure 1.

^d Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Kristallographie und Strukturphysik, Staudtstr. 3, 91058 Erlangen, Germany. Fax: +49-9131-85-25182; Tel.: +49-9131-85-25189; E-mail: Tobias.Unruh@krist.uni-erlangen.de

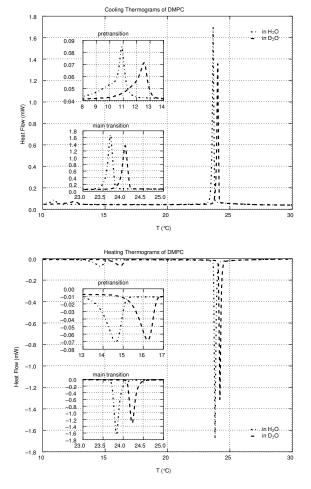


Fig. 1 Differential scanning calorimetry (DSC) measurements of DMPC in H_2O (dash-dotted lines) and D_2O (dashed lines). Shown are the cooling scan (top) and heating scan (bottom). The insets show enlarged versions of the pretransition and main transition peaks.

^{*a*} Technische Universität München, Physik Department E13 and Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Lichtenbergstr. 1, 85748 Garching bei München, Germany. Fax: +49-89-289-14911; Tel: +49-89-289-14922; E-mail: sbusch@ph.tum.de

^b Universitat Politècnica de Catalunya, Grup de Caracterizació de Materials, Departament de Física i Enginyeria Nuclear, ETSEIB, Diagonal 647, 08028 Barcelona, Catalonia, Spain.

 ^c Eidgenössische Technische Hochschule Zürich, Animal Imaging Center
PET, Center for Radiopharmaceutical Sciences of ETH, PSI and USZ, Wolfgang-Pauli-Str. 10, 8093 Zürich, Switzerland.

3 Calculation of the area per molecule

Spherical droplets with radius *r* and diameter $2r = \emptyset$ have a volume of $V = 4/3\pi r^3$, a surface of $S = 4\pi r^2$, and correspondingly $S/V = 3/r = 6/\emptyset \propto 1/\emptyset$. Approximating the density of all components with 1, the volume of spherical droplets in a unit sample volume is given by the concentration of perdeuterated hexadecane, [dHD]. Therefore, the surface area of the emulsion droplets in the same volume is

area
$$\propto \frac{[\text{dHD}]}{\varnothing}$$
 . (1)

As the number of DMPC molecules in the same volume is proportional to the concentration of DMPC in the sample, [DMPC], one finally arrives at

area per molecule
$$\propto \frac{[dHD]}{[DMPC] \cdot \emptyset}$$
 . (2)

This number is only a relatively rough measure for the true value because it assumes that the emulsion droplets are monodisperse and all DMPC molecules are adsorbed to the interface. The formula neglects the surface area occupied by NaGC molecules because the NaGC molecules are water soluble and the amount of NaGC is much lower than the one of DMPC.

4 Fit functions

The fit function used for the determination of the long-range motional component has been discussed in detail before². It is

$$S(Q, \omega) = a \cdot X(Q, \omega) \otimes [A_1(Q) \cdot \delta(\omega) + (1 - A_1(Q)) \cdot L_1(Q, \omega)] \otimes [A_2(Q) \cdot \delta(\omega) + (1 - A_2(Q)) \cdot L_2(Q, \omega)]$$
(3)

where X is discussed in the following, δ is the delta function, and L_1 and L_2 denote Lorentzians. The first term is caused by long-range motions, the two latter ones by localized motions.

4.1 Flow motions

Assuming flow-like motions with a Maxwell-Boltzmann distribution of the flow velocities, *X* is a Gaussian in ω with a standard deviation $\sigma(Q) = v \cdot Q$ where *v* is the most probable flow velocity.

4.2 Diffusion

Assuming diffusion, *X* is a Lorentzian in ω with a half width at half maximum $\Gamma(Q) = D \cdot Q^2$ where *D* is the diffusion coefficient.

References

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- 2 S. Busch, C. Smuda, L. C. Pardo and T. Unruh, *Journal of the American Chemical Society*, 2010, **132**, 3232.