Supplemental Materials by H. Nakahara et al.

The Role of Palmitic Acid in Pulmonary Surfactant Systems by Langmuir Monolayer Study: Lipid-Peptide Interactions

Hiromichi Nakahara[1], Sannamu Lee[1], Yukihiro Shoyama[2], and Osamu Shibata[1,*]

[1]*Department of Biophysical Chemistry, and* [2]*Department of Pharmacognosy,*
Faculty of Pharmaceutical Sciences, Nagasaki International University;
2825-7 Huis Ten Bosch, Sasebo, Nagasaki 859-3298, Japan

APPENDIX

The monolayer ionization degree (α) is determined by the proton concentration at the surface ($[H^+]_s$) and the surface equilibrium constant for the acid group dissociation (K_s):

$$\frac{\alpha}{1-\alpha} = \frac{K_s}{[H^+]_s} \tag{2}$$

If the proton concentration in the bulk ($[H^+]_b$) is known, the surface proton concentration can be calculated using the Boltzmann equation,

$$[H^+]_s = [H^+]_b \exp\left(-\frac{ze\varphi}{kT}\right) \tag{3}$$

where z denotes the charge number of monolayers, e is the elementary electric charge, and φ is the potential difference of the ionic layer. Furthermore, the Gouy-Chapman approach[1] is used to relate φ_0 to the charge density ($\rho \approx \alpha ze/A$) under the condition of NaCl solution at 298.2 K,

$$\varphi_0 = \frac{2kT}{ze}\sinh^{-1}\left(\frac{1.37\alpha}{A\sqrt{c}}\right) \tag{4}$$

where c (in mol/L) is the 1-1 electrolyte concentration. As for the negatively charged monolayer ($z = -1$), the following equation is derived from combining eqs. (2)–(4) .

$$\mathrm{pH_b} = \mathrm{p}K_s + \log\frac{\alpha}{1-\alpha} + 0.87\sinh^{-1}\left(\frac{1.37\alpha}{A\sqrt{c}}\right) \tag{5}$$

Reference

1. E. Maltseva, V. L. Shapovalov, H. Möhwald and G. Brezesinski, *J. Phys. Chem. B*, 2006, **110**, 919-926.

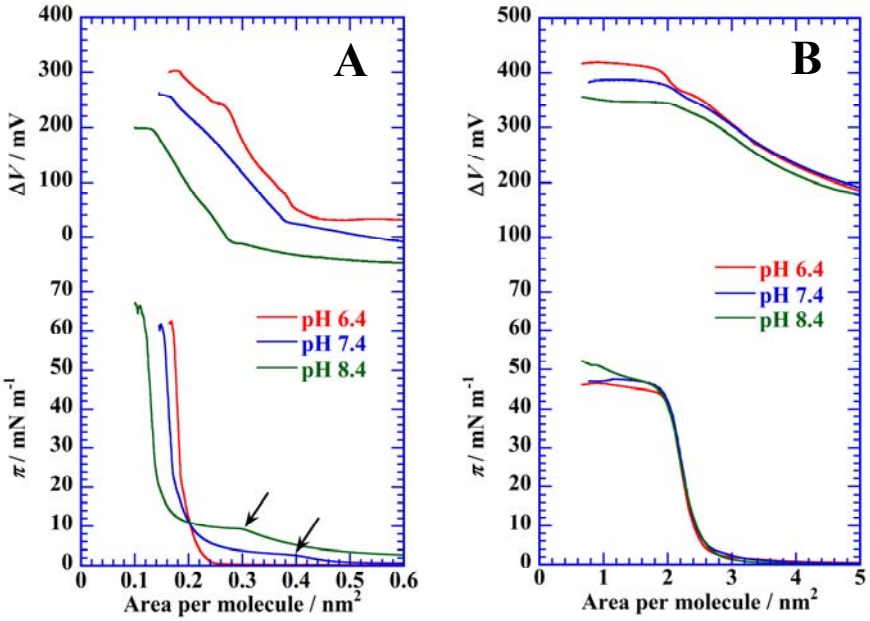

Fig. S1 The π–A and ΔV–A isotherms of (A) PA and (B) Hel 13-5 monolayers on a 0.02 M Tris buffer solution with 0.13 M NaCl at 298.2 K. The subphase pH is prepared to pH 6.4, 7.4, and 8.4.

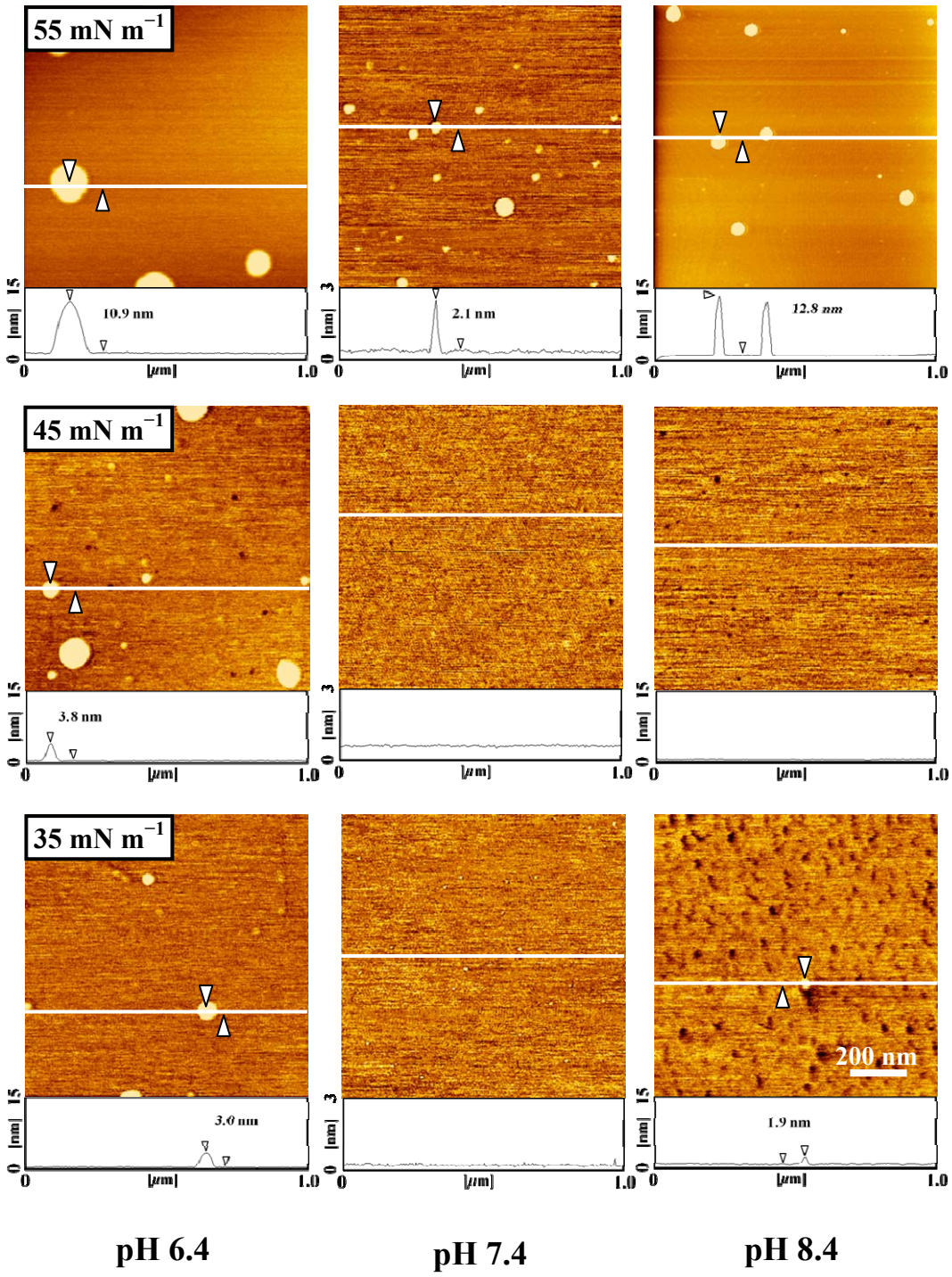

Fig. S2 Typical AFM topographic images of the DPPC/PA(= 90/10, by weight)/Hel 13-5 preparation ($X_{\text{Hel 13-5}}$ = 0.025) at 35, 45, and 55 mN m^{-1} on a 0.02 M Tris buffer solution (pH 6.4−8.4) with 0.13 M NaCl at 298.2 K. All images exhibit LC domains of the ternary monolayer, which are expressed by bright contrast in the FM images. The cross-sectional profiles along the scanning line (white lines) are given just below the respective AFM images. The height difference between the arrowheads is indicated in the cross-sectional profile.

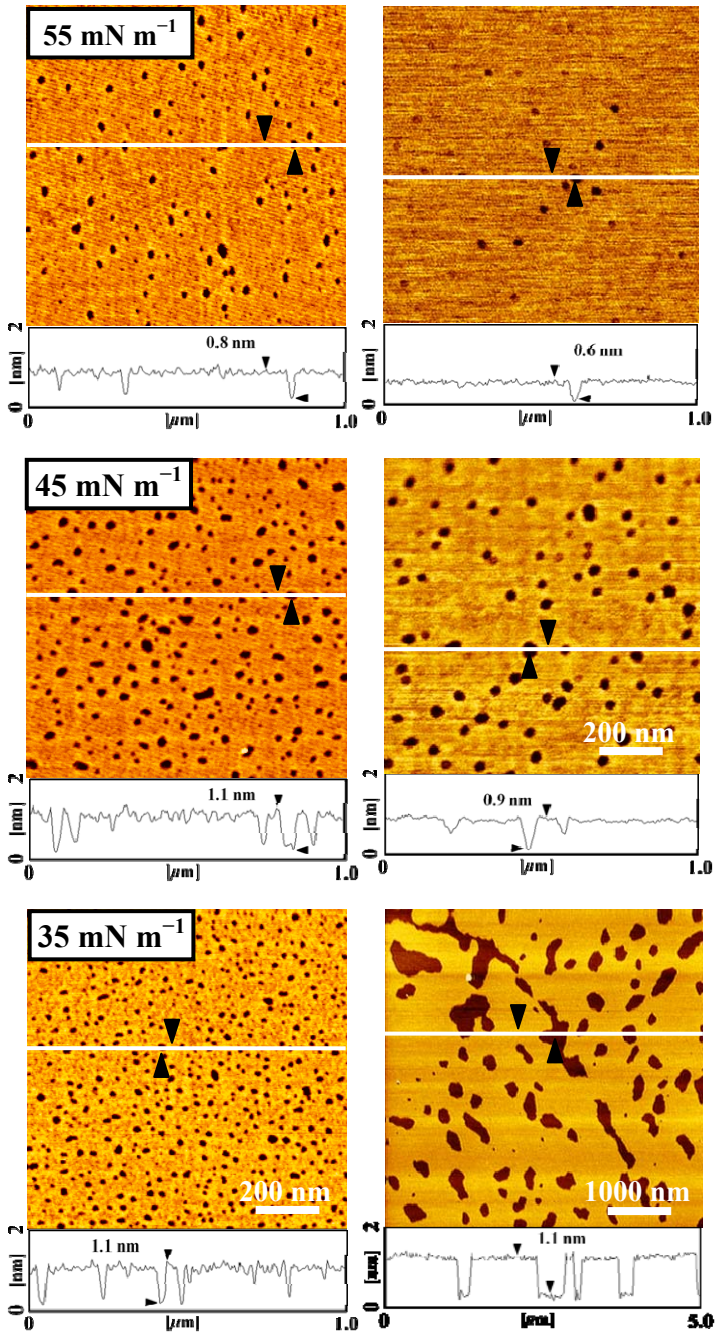

Fig. S3 Typical AFM topographic images of the DPPC/TD(= 90/10, by weight)/Hel 13-5 and DPPC/HD(= 90/10, by weight)/Hel 13-5 preparations ($X_{\text{Hel 13-5}}$ = 0.025) at 35, 45, and 55 mN m^{-1} on a 0.02 M Tris buffer solution (pH 7.4) with 0.13 M NaCl at 298.2 K. All images exhibit LC domains of the ternary monolayer, which are expressed by bright contrast in the FM images. The cross-sectional profiles along the scanning line (white lines) are given just below the respective AFM images. The height difference between the arrowheads is indicated in the cross-sectional profile.

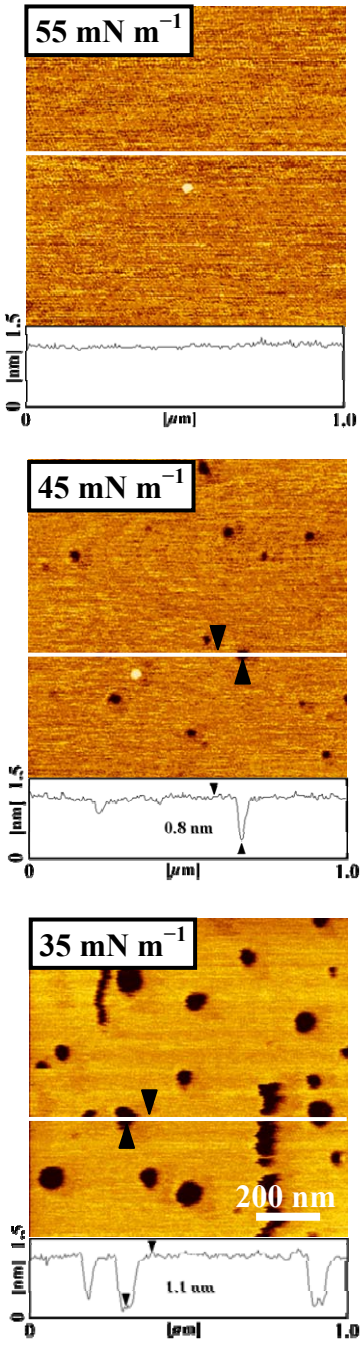

Fig. S4 Typical AFM topographic images of the DPPC/PA(= 90/10, by weight) preparation at 35, 45, and 55 mN m^{-1} on a 0.02 M Tris buffer solution (pH 7.4) with 0.13 M NaCl at 298.2 K. The cross-sectional profiles along the scanning line (white lines) are given just below the respective AFM images. The height difference between the arrowheads is indicated in the cross-sectional profile.