

Electronic Supplementary Information

Protegrin interaction with lipid monolayers: Grazing incidence X-ray diffraction and X-ray reflectivity study

Frances Neville, Yuji Ishitsuka, Chris S. Hodges, Oleg Konovalov, Alan J. Waring, Robert Lehrer, Ka Yee C. Lee,^b and David Gidalevitz

1.Example of Bragg rod and Bragg peak profiles

(Top) Bragg rod profiles.

Top left profile is of the Bragg rod profile corresponding to the $\{11\}^a$ lattice and the top right profile corresponds to the $\{02\}^a$ lattice. The sharp peak observed around $q_z = 0.01 \text{ \AA}^{-1}$ is due to interference of rays diffracted down and subsequently reflected back up by the interface. The $\{11\}^a$ lattice Bragg rod data were fitted with a Gaussian to determine the maximum rod value which was used to calculate the tilt value. In this case the

(Bottom)

Corresponding Bragg peak profile.

The (h,k) reflection assignment is indicated on the two data sets.

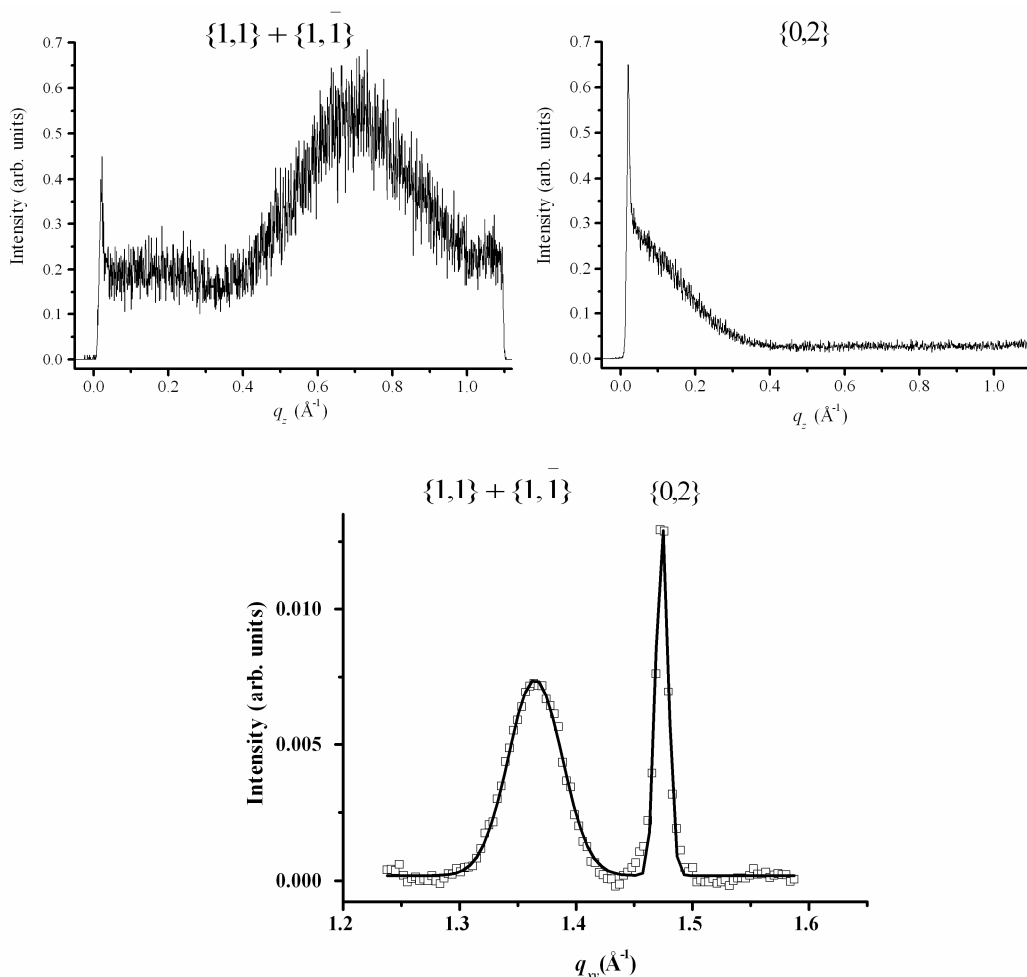


Fig.S1. Grazing incidence X-ray diffraction spectrum of DPPC monolayer at 30 mN m^{-1} surface pressure over Dulbecco's phosphate buffered saline solution.

^a "11" and "02" are used to denote (hk) for a set of Bragg rods with equal in-plane components which cannot be resolved from the GIXD data. In this case data are calculated using the rectangular unit cell, thus $\{11\}$ lattice means $\{(11), (1\bar{1}), (\bar{1}1), (\bar{1}\bar{1})\}$ and $\{02\}$ means $\{(02), (0\bar{2})\}$.

2. Comparison of L_1 XR fitting values and those obtained from tilt angles

Experiment	$L_1 / \text{\AA}$ (XR fitting)	Roughness $_{L_1}$ $\sigma / \text{\AA}$	Tilt ($^\circ$)	$L_1 / \text{\AA}$ (from tilt angle)
DPPC 20 mN m $^{-1}$	12.6	4.0	49	12.6
DPPC 20 mN m $^{-1}$ + PG-1	12.5	4.2	29	16.6
DPPG 20 mN m $^{-1}$	13.9	N/A	33	16.1
DPPC 30 mN m $^{-1}$	15.2	3.3	30	16.6
DPPC 30 mN m $^{-1}$ + PG-1	16.1	5.5	30	16.6
DPPG 30 mN m $^{-1}$	18.1	3.7	27	17.1
DPPG 30 mN m $^{-1}$ + PG-1	14.9	5.2	32	16.3