

Contents

Introduction	1
1 Elements of lipid bilayer fusion	5
1.1 Lipids	5
1.2 Phospholipid mesophases	7
1.3 Bilayer fusion pathways	10
1.4 Interaction potentials between lipid bilayers	11
1.5 Continuum theory and simulations of stalks	14
2 X-ray diffraction on lipid mesophases	17
2.1 Fundamentals of X-ray diffraction	17
2.2 Oriented samples	20
2.3 Experimental techniques	22
2.3.1 X-ray reflectivity	22
2.3.2 Grazing-incidence x-ray diffraction	23
2.3.3 Powder diffraction	25
2.4 Intensity correction factors	26
2.5 The phase problem	29
2.6 Resolution	31
3 Lyotropic lipid polymorphism	35
3.1 Hydration control by water vapour	35
3.2 Experimental	37
3.2.1 Sample preparation	37
3.2.2 Sample environment	38
3.2.3 In-house small-angle x-ray scattering setup	39
3.2.4 Phase diagram determination	41
3.3 Results	41
3.3.1 Characteristic diffraction patterns	41
3.3.2 Phase diagrams	42
3.3.3 Indexing of Diffraction patterns	48
3.4 Conclusions	55
4 Bilayer structure and interactions	57
4.1 Electron density profiles	57
4.2 Osmotic stress method	58
4.3 Motivation of our work	61
4.4 Experimental	62
4.4.1 X-ray reflectivity Instrument	62
4.4.2 Measurements	63
4.4.3 Data reduction	63
4.4.4 Fourier Synthesis of electron density profiles	66
4.4.5 Phase retrieval: The swelling method	66
4.5 Results and Discussion	72

4.5.1	Effects at close bilayer separation	72
4.5.2	Bilayer structure	72
4.5.3	Hydration force parameters	74
4.5.4	Hydration barrier for membrane fusion	79
4.6	Conclusions	81
5	Structure determination of stalks	83
5.1	Data collection and reduction	83
5.1.1	Synchrotron GIXD experiments	83
5.1.2	X-ray reflectivity experiments	93
5.1.3	Powder diffraction experiments	94
5.1.4	Combination of different X-ray geometries	98
5.2	Solving the phase problem	98
5.3	Results	106
5.4	Discussion	112
5.5	Conclusions	113
6	Analysis of the 3d electron density of stalks	115
6.1	Structural parameters of the stalk phase	115
6.1.1	Definitions	115
6.1.2	Results	117
6.2	Electron density isosurface analysis	119
6.2.1	Motivation	119
6.2.2	Differential geometry of implicit surfaces	121
6.2.3	Implementation	122
6.2.4	Results	124
6.3	Discussion and comparison to continuum theory	131
6.3.1	General remarks	131
6.3.2	Possible limitations of continuum theory	131
6.3.3	Comparison to continuum models	132
6.4	Conclusions	134
7	Summary	135
A	Appendix	137
A.1	Triplet relationship	137
A.2	Crystallographic data and swelling diagrams	139
A.3	Gauss-Bonnet theorem applied to stalks	156
A.4	MATLAB code: Examples	158
	References	171
	List of publications	183
	Danksagung	185
	Curriculum Vitae	187