

Contents

1	Introduction	1
	References	5
2	Theoretical Background	9
2.1	Lipid Membranes	9
2.1.1	Physics of Lipids and Lipid Membranes	9
2.1.2	Inter-Membrane Interactions	12
2.1.3	Mechanics of Solid-Supported Membrane Multilayers	16
2.1.4	Membrane Models	19
2.2	Principles of X-Ray and Neutron Scattering	23
2.2.1	Basic Principles	23
2.2.2	Specular Scattering	26
2.2.3	Off-Specular (Diffuse) Scattering	30
	References	36
3	Materials and Methods	39
3.1	Materials	39
3.1.1	DPPC and Synthetic Glycolipids	39
3.1.2	Lipopolysaccharides	41
3.1.3	Chemicals and Buffers	42
3.2	Preparation Methods	43
3.2.1	Preparation of Solutions/Suspensions	43
3.2.2	Preparation of Solid-Supported Membrane Multilayers	44
3.2.3	Preparation of Rough Mutant LPS Monolayers at the Air/Water Interface	45
3.2.4	Preparation of Solid-Supported PAOLPS Monolayers	45
3.3	Scattering Techniques	46
3.3.1	X-Ray Scattering	46
3.3.2	Neutron Scattering	48
3.3.3	Sample Environments	50
	References	52

4 Theoretical Modeling	55
4.1 Determination of Mechanical Properties of Interacting Membranes	55
4.1.1 Membrane Displacement Correlation Functions	55
4.1.2 Calculation of Specular and Off-Specular Scattering Signals	57
4.1.3 Summary of Sect. 4.1	64
4.2 Electrostatic Interactions between Charged Lipid Membranes	64
4.2.1 A Single Charged Surface in an Electrolyte	65
4.2.2 Two Charged Surfaces in an Electrolyte	66
4.2.3 The Weak-Overlap Approximation	68
4.2.4 Summary of Sect. 4.2	69
4.3 Interpretation of X-Ray Fluorescence Signals	69
4.3.1 Calculation of Illumination Profiles	70
4.3.2 Calculation of X-Ray Fluorescence Intensities	73
4.3.3 Summary of Sect. 4.3	77
References	77
5 Inter-Membrane Interactions and Mechanical Properties of Membranes Composed of Synthetic Glycolipids	79
5.1 Influence of Molecular Structure: Cylindrical and Bent Saccharides	79
5.1.1 Phase Transitions of Glycolipid Membranes	79
5.1.2 Modulation of Inter-Membrane Interactions via Saccharide Conformation	82
5.1.3 Influence of Saccharide Conformation on Membrane Mechanics	83
5.1.4 Summary of Sect. 5.1	87
5.2 Role of Specific Saccharide-Saccharide Interactions in Membrane-Membrane Contacts	88
5.2.1 Influence of LewisX Trisaccharides on Inter-Membrane Interactions	89
5.2.2 Specific Saccharide-Saccharide Interactions under Compressional or Tensile Stress	90
5.2.3 Influence of LewisX on the Mechanics of Membrane Multilayers	95
5.2.4 Summary of Sect. 5.2	97
References	98
6 Structure and Mechanical Properties of Bacteria Surfaces	101
6.1 Influence of Lipopolysaccharide Structure and Divalent Cations on the Mechanics of LPS Multilayers	101
6.1.1 Influence on Inter-Membrane Interactions	102
6.1.2 Influence on Mechanical Properties	104
6.1.3 Summary of Sect. 6.1	107

6.2	Influence of Divalent Cations on the Conformation of Wild-Type Lipopolysaccharides	107
6.2.1	Effect of Divalent Cations: Electron Density Profile of LPS Monolayers	108
6.2.2	Modeling of LPS Saccharide Conformation by Coarse-Grained Monte Carlo Simulations	110
6.2.3	Summary of Sect. 6.2	112
6.3	Concentration Profiles of Monovalent and Divalent Cations at Bacteria Surfaces	113
6.3.1	Influence of Divalent Cations on Molecular Interactions in Langmuir Monolayers of LPS Re	113
6.3.2	Influence of Divalent Cations on Electron Density Profiles of LPS Re Monolayers	114
6.3.3	Ion Concentration Profiles at LPS Re Monolayers	116
6.3.4	Modeling of Ion Concentration Profiles at LPS Re Monolayers by Coarse-Grained Monte Carlo Simulations	120
6.3.5	Summary of Sect. 6.3	121
	References	122
7	Conclusions	125
8	Outlook	127