

Contents

1	Introduction	1
2	Computer Simulation Methods	7
2.1	Preliminary Remarks	7
2.2	Molecular Dynamics	8
2.2.1	The Equation of Motion in a Classical Many-Particle System	8
2.2.2	Numerical Aspects	9
2.3	Monte Carlo Methods	12
2.3.1	The Modified Metropolis Algorithm in the Grand Canonical Ensemble	12
2.3.2	The Modified Metropolis Algorithm in the Isostress-Isostrain Ensemble	16
3	Equilibrium Properties of Vicinal Phases	23
3.1	Preliminary Remarks	23
3.2	Experimental Background	24
3.2.1	The Surface Force Apparatus	24
3.2.2	Total Internal Reflection Microscopy	27
3.2.3	The Atomic Force Microscope	28
3.3	Models in Computer Simulation Studies	29
3.3.1	Model I: Structured Soft Wall	31
3.3.2	Model II: Structureless Soft Wall	34
3.3.3	Model III: Structureless Hard Wall	34
3.3.4	Model IV: Infinitesimally Rough Hard Wall	35
3.4	Computer Simulation Results	36
3.4.1	Connecting with Experiments: The Solvation Force	36
3.4.2	Vicinal Phase Structure	40
3.4.3	Results for Other Model Systems	48

3.5	Numerical Approaches Besides Computer Simulations. . .	51
3.5.1	The Born-Green-Yvon Equation	51
3.5.2	Density Functional Theory	53
4	Phase Transitions in Vicinal Phases.	57
4.1	Preliminary Remarks	57
4.2	Capillary Condensation	58
4.2.1	Sorption Experiments	58
4.2.2	Application of Density Functional Theory to Capillary Condensation	59
4.2.3	Hysteresis in Computer Simulations: A Critique	62
4.2.4	The Phase Diagram	68
4.2.5	Wetting.	69
4.3	Shear Melting of Solid Vicinal Phases.	70
4.3.1	Introduction to Shear Melting Experiments.	71
4.3.2	Computer Simulation of Shear Melting	74
4.3.3	Critical Evaluation of the Relation Between Computer Simulation and Laboratory Experiment	92
5	Time-Dependent Properties	97
5.1	Preliminary Remarks	97
5.2	Self-Diffusion in Vicinal Phases	99
5.2.1	Macroscopic and Microscopic Description of Self-Diffusion	99
5.2.2	Inhomogeneity and Anisotropy	107
5.2.3	The Influence of Wall Structure	109
5.3	Anomalous Diffusion.	111
5.3.1	The Role of Spatial Hindrance	111
5.3.2	Fractional Dimension of Self-Diffusion and Its Relation to Shear Melting	113
5.3.3	In-Plane Anisotropy of Atomic Motion	119
5.4	Transport Phenomena and Non-Equilibrium Molecular Dynamics Calculations.	120
6	Summary	123
	References	127