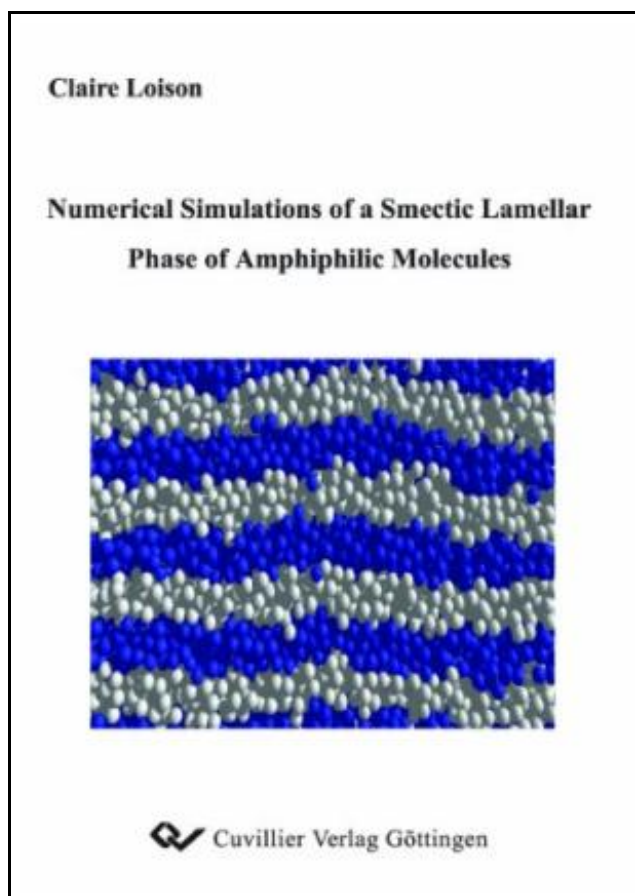


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Cuvillier Verlag Dez 2005, 2005. Taschenbuch. Book Condition: Neu. 208x147x12 mm. Neuware - This thesis deals with the liquid crystalline lamellar phase L built by amphiphilic molecules in aqueous solutions, and its interaction with macromolecules. We perform molecular dynamics simulations to study thermal fluctuations and defects appearing in a stack of parallel amphiphilic bilayers separated by layers of solvent. The idealized, coarse-grained model represents the solvent with soft spheres and the amphiphiles with bead-and-spring tetramers (two solvophilic beads and two solvophobic beads). The algorithm used for this thesis describes the lamellar phase in the isobaric isothermal ensemble without surface tension ($N, P, T, = 0$). First, we verify that the model exhibits a liquid-crystalline lamellar phase, which we characterize. In a second part, we study the elasticity of this smectic lamellar phase. The position fluctuation spectra of the bilayers are computed, and compared to the predictions of the Discrete Harmonic (DH) theory for the elasticity of smectic phases. The bilayer fluctuations observed in the simulation of a stack of fifteen bilayers are well described by the DH-theory, so that the two elastic constants - the bending rigidity K_c and the smectic compressibility modulus B - can be computed. Then, we investigate the point defects appearing in the smectic because of thermal fluctuations. It turns out that transient pores spontaneously nucleate in the bilayers of the lamellar phase. On the contrary, necks and passages between the bilayers are rarely detected. The size and shape distributions of the pores are investigated. The relationship between their area a and their contour length c is well described by the scaling law $a \propto c^{2/3}$ - the same scaling as two dimensional closed random walks. Additionally, the surface tension is zero. Therefore we consider that the energy of a pore depends explicitly only on the contour length of...



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