

**LAMELLAR PHASE OF SHORT AMPHIPHILES: MOLECULAR
DYNAMICS SIMULATIONS COMPARED TO SIMPLE
MESOSCOPIC MODELS**

CLAIRE LOISON^{1*}, FRIEDERIKE SCHMID² and MICHEL MARESCHAL³
¹Max Planck Institut für Chemische Physik Fester Körper, Nöthnitzerstrasse 40,
D01187 Dresden, Germany, ²Fakultät fuer Physik, Universität Bielefeld,
Universitätstraße 25, D33615 Bielefeld, Germany, ³Université Libre de
Bruxelles, Faculté des Sciences, CP231, Boulevard du Triomphe,
B1050 Brussels, Belgium

We review recent molecular dynamics simulations of thermally activated undulations and defects in the lamellar $L\alpha$ phase of a binary amphiphile-solvent mixture, using an idealized molecular coarse-grained model: Solvent particles are represented by beads, and amphiphiles by bead-and-spring tetramers. The amphiphilic membranes self-assemble into a lamellar stack of amphiphilic bilayers separated by solvent layers. At a solvent bead fraction of 20% and sufficiently low temperature, the amphiphiles self-assemble into a highly oriented lamellar phase. Our study aims at comparing the structure of this phase with the predictions of the elastic theory of thermally fluctuating fluid membrane stacks [Lei, N. *et al.* **J. Phys.** **II** 5 (1995) 1155]. We suggest a method which permits to calculate the bending rigidity and compressibility modulus of the lamellar stack from the simulation data [Loison, C. *et al.* **J. Chem. Phys.** 119 (2003) 13138]. The simulation results are in reasonable agreement with the theory. We focus then on the particular case of tension less membranes, in which pores spontaneously appear because of thermal fluctuations [Loison, C. *et al.* **J. Chem. Phys.** 121 (2004) 1890]. Their spatial distribution is similar to that of a random set of repulsive hard discs. The size and shape distribution of individual pores can be described satisfactorily by a simple mesoscopic model, which accounts only for a pore independent core energy and a line tension penalty at the pore edges. In particular, the pores are not circular: their shapes are fractal and have the same characteristics as those of two dimensional ring polymers. Finally, we study the size-fluctuation dynamics of the pores, and compare the time evolution of their contour length to a random walk in a linear potential. Finally, we discuss implications for polymer-membrane systems [Loison, C. *et al.* **Comp. Phys. Comm.** (2005), condmat/0501073, in press].

* E-mail: loison@cpfs.mpg.de