Chirality and Curvature in the Gyroid Mesophase

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1. Amphiphile mesophases
2. Membrane model
3. Lattice Boltzmann modelling
4. Domain growth law
5. Chiral domains
6. Summary

What is an amphiphile?

Like a soap molecule

- Composed of oil-loving and water-loving parts

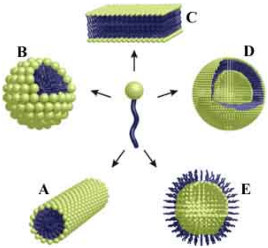

Image from http://www.vcbio.sci.kun.nl/fesem/applets/amphiphiles/

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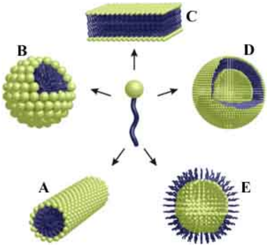

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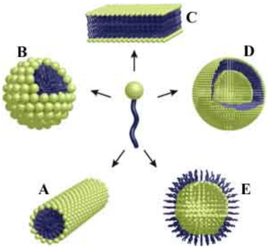
- Diblock copolymers are similar



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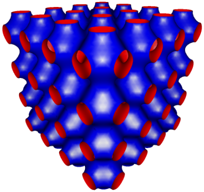
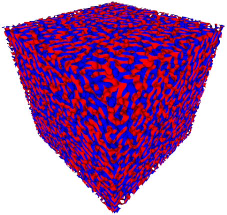
Bicontinuous phases

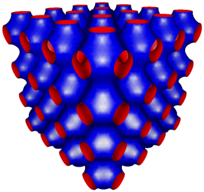
- Continuous, interpenetrating networks of channels

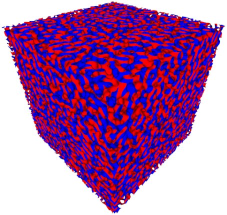




Bicontinuous phases

- Continuous, interpenetrating networks of channels
- Can self-assemble

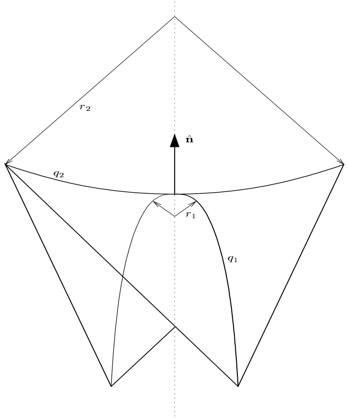




Membrane model

- Surfactant interactions extremely complicated
- Simplified model treats surfactant layer as curved membrane

Membrane model



Mean curvature $H = \frac{1}{2}(c_1 + c_2)$; Gaussian curvature $K = c_1 c_2$

Canham-Helfrich Hamiltonian

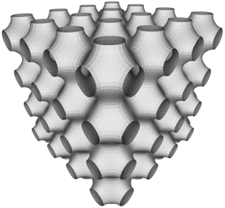
$$E_{\mathrm{curv}} = \int \left[2\kappa\left(H - H_0\right)^2 + \bar{\kappa}K\right] \mathrm{d}S$$

- Spontaneous curvature H_0
- Splay curvature modulus κ
- Saddle splay modulus $\bar{\kappa}$

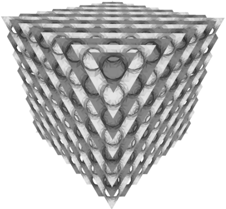
Gaussian curvature term depends *only* on topology, due to Gauss-Bonnet theorem:

$$\bar{\kappa}\int K \mathrm{d}S = 2\pi\chi$$

Cubic TPMS phases



P surface



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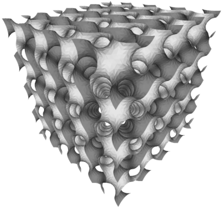

G surface

Ternary amphiphilic LB

- Model of Chen, Boghosian, Coveney, and Nekovee: *Proc. R. Soc. London A* **456**, 2043 (2000)

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- Amphiphile particles modelled as dipoles, with orientational degrees of freedom.
- Grid computing techniques used to run large simulations to avoid finite size effects

Gyroid formation dynamics

Three stages:

- Rapid phase segregation and formation of channels

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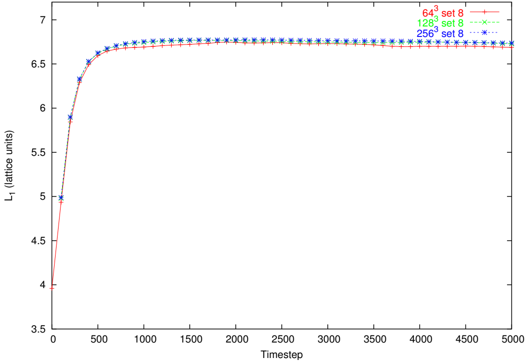
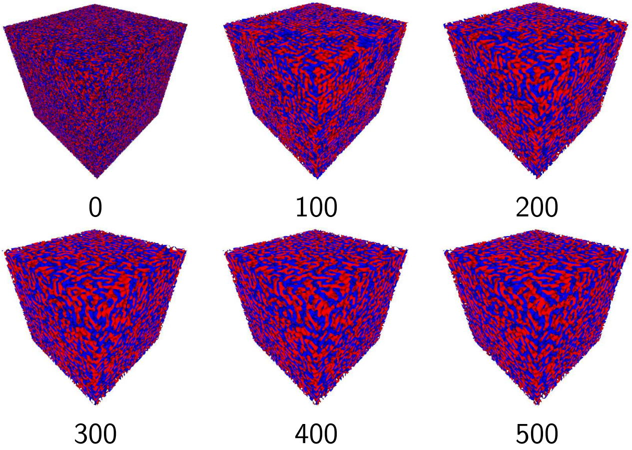
- Gyroid domain growth

Rapid phase segregation



Rapid phase segregation



Characterization of gyroid regions

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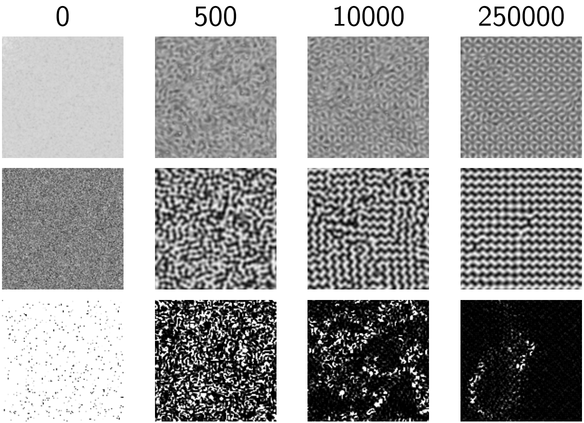
- Triangulate interface
- Calculate curvature at each vertex
- Bin results back to find interfacial curvature per lattice site

Formation of domains



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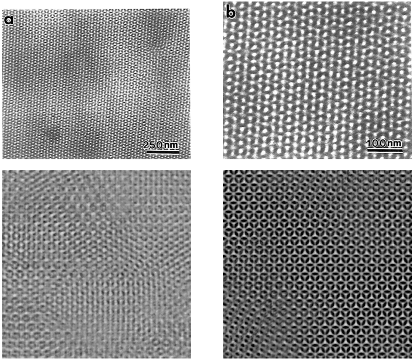
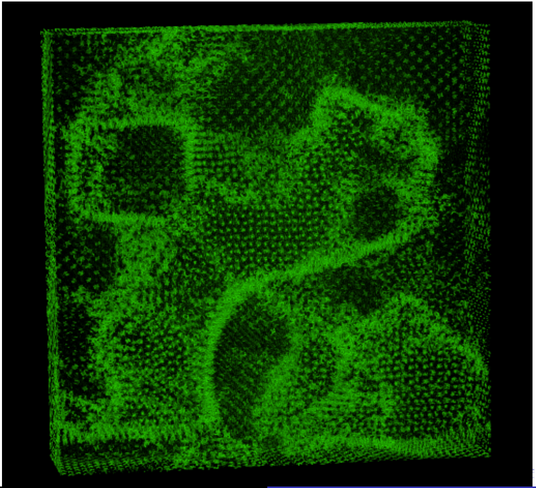
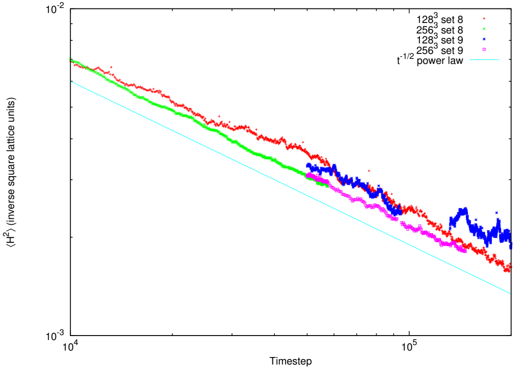


TEM images a,b from Laurer *et al*, *Macromolecules* **30** 3938 (1997).

Gyroid domains



Domain growth law

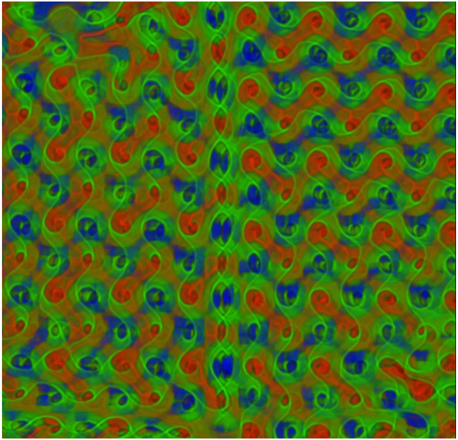


$$\langle H^2 \rangle \simeq At^{\lambda}, \text{ where } \lambda = -0.48 \pm 0.04$$

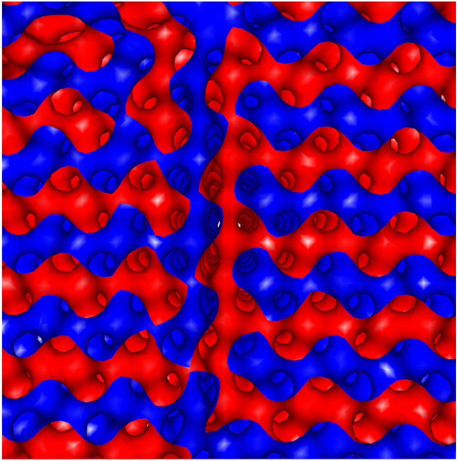
Diffusive growth?

- Suppose the main contribution to $\langle H^2 \rangle$ is from domain walls of similar thickness λ
- Consider a system of volume V, containing many gyroid domains of length scale $L_1(t) \sim t^n$
- Area of single domain is $A_1 \sim t^{2n}$; volume is $V_1 \sim t^{3n}$
- Total number of domains in volume is V/V_1, so $N \sim t^{-3n}$
- Total surface area of domains $A \sim N(t)A_1(t) \sim t^{-n}$
- Volume of domain walls scales as $V_{\mathrm{dom}} \sim \lambda A \sim t^{-n}$

Domain wall



Chiral domains



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- Surface-averaged mean curvature gives a measure of defect density
- Curvature appears to scale as $t^{-1/2}$ at late times, possibly indicating diffusive behaviour
- Domains may be differently oriented or have different chirality.

Thanks

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