Monte Carlo simulation of polydisperse spheres on a spherical surface

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Abstract: In this project the Monte Carlo method has been applied to simulate the self-assembly of colloidal spherical silica particles on latex spherical nanodroplets. The information supplied by this simulation is complementary to the experimental data and has been used to determine whether thermodynamic equilibrium has been reached and to study the effect of polydispersity on the self-assembled structure.

1. Experiment: spheres on a spherical surface

(C. Colard and S. Bon)

This project has been inspired by this self-assembled structure:

- polymeric core
- silica particles covering
- polydisperse
- uncharged

which has been modelled as follows:

- Polar coordinates
- Polydispersity
- Gaussian distribution
- Force Field: modified Lennard-Jones potential

2. Delaunay triangulation on the spherical surface

This is a method to describe the geometry of a set of points on a spherical surface.

Definition:
Each triangle of the triangulation should satisfy the Delaunay condition: no vertex should be located inside the circumsphere of any triangle.

How to triangulate:
- for every sphere identify a vertex on a unitary surface
- search for nearest nodes to define a set of triangles
- flipping technique to satisfy Delaunay condition

3. Network defects

Definition:
A sphere whose center belongs to \( n_d \) triangles is defined as an \( n_d \)-fold disclination.

Point Defects
- Isolated points with \( n_d \neq 6 \)

Scars
- Line defects: alternation of \( n_d = 5 \) and \( n_d = 7 \)

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- The extension of the network formed by \( n_d \neq 6 \) is a function of the polydispersity.

The simulation result (right) is consistent with the experimental observation and this allows us to state that the system has reached thermodynamical equilibrium. Other useful information can be extracted by applying the Delaunay triangulation to a set of simulated structures (left).

A plot of the fraction of \( n_d \)-dislocations as a function of the polydispersity (right), shows that the experimental system lie in an intermediate position with respect to two different behaviors, one associated with monodispersity and one with high polydispersity.

4. Radial distribution function

To understand what happens in the two extreme situations, monodisperse and highly polydisperse, we used the following:

Defect pair distribution function

\[
G_{\alpha\beta}(d) = \frac{N_{\alpha\beta}^\text{sim}(d)}{A \cdot S(d) \cdot \rho_\alpha \cdot \rho_\beta}
\]

showing that the short range order of the monodisperse case is completely lost and we have a totally new structure.

5. Void space distribution

One open question is whether or not a polydisperse self-assembled structure can act as a molecular cage. To answer to this question, the void space distribution (i.e. the pore size distribution) has been studied.

The polydispersity does not seem to be critical for the pore size distribution.

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