DRYING-MEDIATED SELF-ASSEMBLY OF NANOPARTICLES

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When a liquid containing nanoparticles evaporates, many fascinating transitory structures can form [1]. While certain experimental results can be explained using thermodynamic arguments alone, drying-assisted aggregation of nanoparticles is, in principle, a non-equilibrium phenomenon [2]. Understanding this evolution towards a new equilibrium state at a microscopic level is the first step in a systematic design of interesting and useful morphologies.

Here, we present a coarse-grained lattice-gas model in two- and three-dimensions of this dynamical self-assembly that accounts for spatial and temporal patterns observed in thin film experiments [2,3]. Simulations of this model also predict potentially useful network structures that have not yet been explored. We focus on two distinct mechanisms of pattern formation, corresponding to heterogeneous (Fig. 1) and homogeneous (Fig. 2) limits of evaporation dynamics. Our results show how different choices of solvent, nanoparticle size and identity, and thermodynamic state give rise to various aggregate morphologies.

References:

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[2] E. Rabani, D.R. Reichman, P.L. Geissler, and L.E. Brus, "Drying-Mediated Self-Assembly of Nanoparticles", *Nature* **426**, 271-274 (2003).

[3] C.G. Sztrum, O. Hod, and E. Rabani, "Self-Assembly of Nanoparticles in Three-Dimensions: Formation of Stalagmites", s*J. Phys. Chem.* B, **109**, 6741-6747 (2005).

Figures:

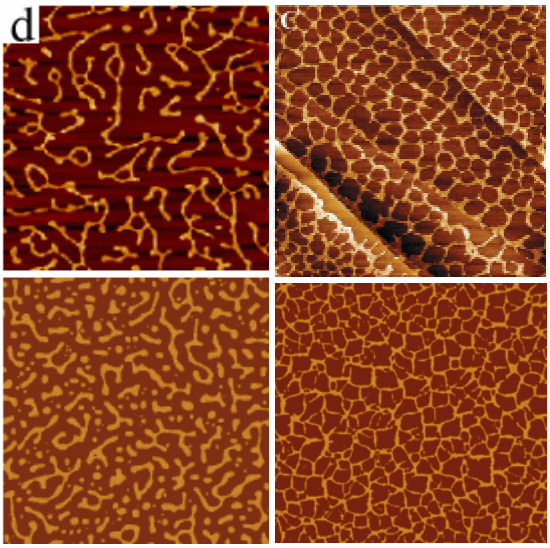

Fig 1: Self-assembled morphologies for heterogeneous evaporation. Experiments and theory are shown in the upper and lower panels, respectively.

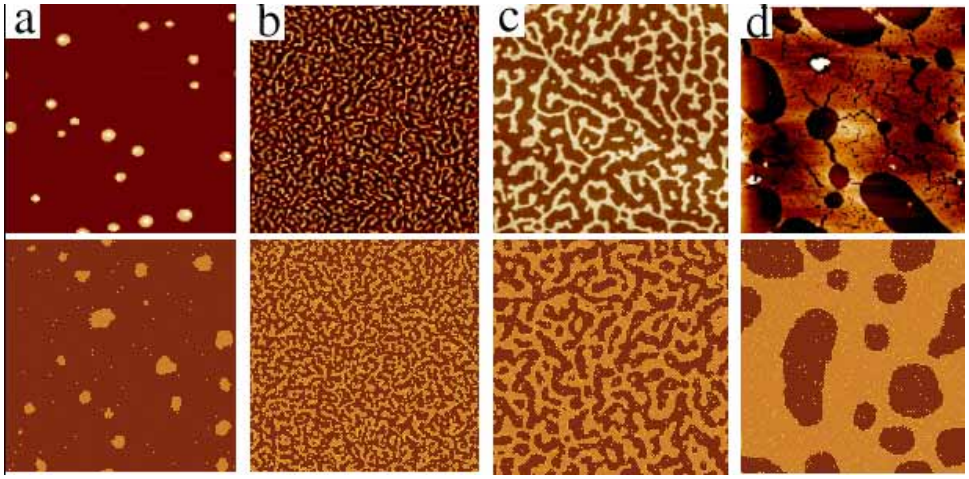

Fig. 2: Self-assembled morphologies at different nanoparticle coverage for homogeneous evaporation. Note the agreement between experiments (upper panels) and theory (lower panels).