Sublimation in colloidal crystals

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Abstract

We are studying colloid polymer systems using the Asakura-Oosawa depletion model. For small interaction distances, the AO model exhibits a crystal to gas phase transition. We used crystals formed by colloids of two sizes. The were then placed into a higher potential field where the began to sublimate, such that the number of monomers N_m was proportional to $t^{2/3}$.

Asakura-Oosawa Potential

The Asakura-Oosawa model consists of two types of particles. The particles do not interact directly. The only limitation on the motion of the particles is that the particles cannot overlap. This condition is defined as limiting the center of mass of a particle to a distance at least one radius away from the edge of any other particle. This creates a depletion zone around the colloidal particle. If the there are two types of particles, a large particle and a small particle, then the entropy of the system can be minimized by minimizing the volume of the depletion zone. The total area of the depletion zone decreases when the large particles are grouped together (Figure 1).

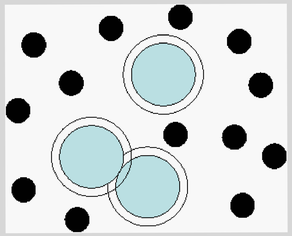


Figure 1

This interaction potential can be described by

$$f(r) = \frac{1}{r^{36}} + a_1(1 + a_2 r + a_3 r^3)$$

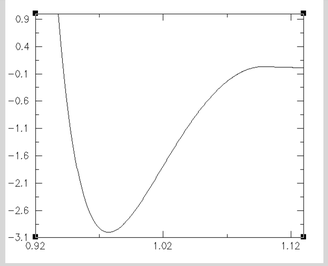


Figure 2

So the AO interaction is a potential well, with a range equal to the radius of the smaller particle. At distances greater than one small radius, there is no interaction between particles.

The parameters of the simulatjon are xi, the ratio of the large particle radius to the small particle radius, and the magnitude of the well depth in terms of kT (the boltzmann constant and a temperature). The crystals used in this simulation were all formed under the influence of a 4kT potential.

The phase diagram(Figure 3) relies on three parameters: temperature, the interaction range of the potential and volume fraction of the colloidal particles.

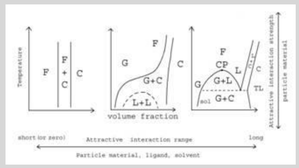


Figure 3

The simulations described here all are described by the middle phase diagram. The volume fraction of the colloids is small enough however, that only crystal to gas transitions occur. This limit is called the protein limit.

Sublimation in Two Dimensions

Sublimation under the influence of a depletion potential in two dimensions is understood. Figure 4 shows a sublimating crystal.

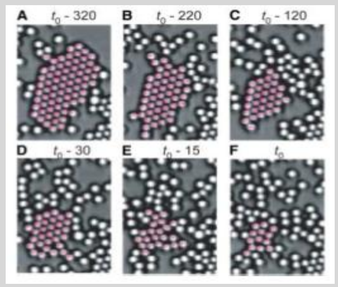
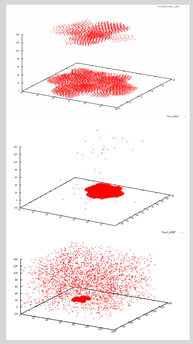


Figure 4

In two dimensions, as the crystal heats up, the outer layer of the crystal loses structure, becoming a transient liquid. Then particles sublimate out of the liquid.

Sublimation in Three Dimensions



To the left and below are four graphs showing a sublimating crystal at t=0, t=50, t=5000 and t=10000.

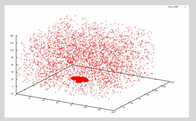
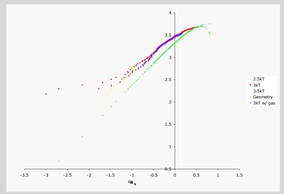


Figure 5

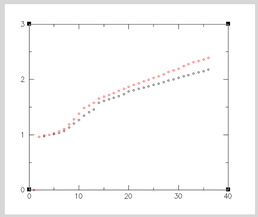


To the left in figure 6 is a graph showing the number of monomers plotted against the change in the radius of gyration for various systems.

Figure 6

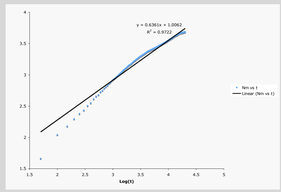
The green line describes the sublimation of a sphere that lost particles uniformly from the surface. The other colors show the results of the simulation at different energies. So the green line seems to work well as an explanation for the geometry of sublimation.

Below is a graph showing the average distance between a particle close to the surface of the crystal and its first 36 nearest neighbors. The black line shows the the distances at t=0 and the red line shows the distances t=30,000. Some expansion is expected in a sublimating crystal. However, this relatively small expansion means that most of the lost volume is due to the emitted monomers.



The linear nature of the graph in the later stages indicates that there is little structure at the edge of the crystal.

Figure 7



The crystal exhibits scaling as it sublimates such that the number of monomers N_m goes like $t^{2/3}$.

Conclusions/Future Research

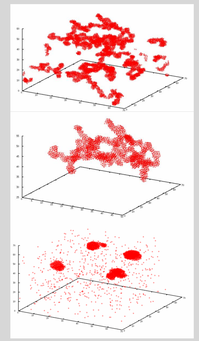
The scaling relationship from above needs to be explain. One possible explanation is that the sublimation rate depends on the surface area of a crystal and the AO potential such that

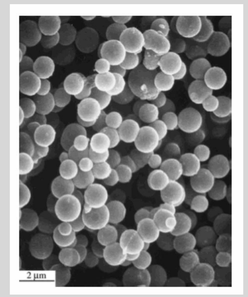
$$\frac{dN}{dt} = aR^2 - bR^3$$

$$N^{\frac{1}{3}} = \frac{a}{b} - \frac{A}{b} e^{-\frac{bt}{3}}$$

This formula is a promising, but the values of *a* and *b* need to be determined before the formula can be fully evaluated.

Real World Applications





On the right, an AO potential is used to create a gel. The largest cluster is then removed and placed in a higher potential. This gives rise to the microsphere droplets in the bottom frame. This method has been used to create microsphere droplets of insulin, which is crucial in treating diabetes.

References

Imaging the Sublimation Dynamics of Colloidal Crystallites. J. R. Savage, D. W. Blair, A. J. Levine, R. A. Guyer, A. D. Dinsmore *Science* 3 November 2006: Vol. 314. no. 5800

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