Home > A Long and Winding Road

A Long and Winding Road [1]

Submitted by Gabriel Ivan Vega Bellido [2] on 5 August 2017 - 11:01pm

[2]

Me, the model system, and a probability distribution of orientations between bonded particles summarizing the range of possible structures.

Self-Assembly of magnetic colloids with shifted dipoles via Brownian Dynamics Simulations.

To many people this might seem like a strange and intimidating array of fancy science words, but to me they are a very important array of fancy science words. This is the name of the project that has occupied me for around a year and a half, one which was initially an entirely alien concept to me. Herein I will attempt to make that title somewhat less intimidating.

Magnetic colloids are precisely what they sound like, colloids with magnetic properties. Wherever there are magnetic properties, one is sure to find a dipole involved, a dipole being that inseparable pair of magnetized poles which characterize all magnets. When dealing with the spherical particles that compose a colloid, like is the case for this project, the easiest way to imagine the dipole that gives the particle its magnetic properties is by sitting it at the very center of the particle. The main concept of my work lies in what happens when you start laterally shifting that dipole towards the surface of the particle. What interests me are the ways in which the shifting of the dipole affects the aggregation (Or Self Assembly) of these particles. The shift is scaled using the radius of the particle, taking on values from 0 at the center of the particle, and 1 at the surface. The final, and perhaps most intimidating, part of my title is the "*Brownian Dynamics Simulations*". At first this was also what most scared me, since my background in heavy duty

coding is non-existent, but we'll stick to the basics of this phrase. Brownian motion is the phenomenon by which particles submerged in water move about in a random manner due to collisions with the water molecules, named after Robert Brown who first observed it, though the explanation for it was given by Albert Einstein nearly 8 decades later. Hence a Brownian Dynamics Simulation is one in which the movement caused by Brownian motion is considered as a random force which affects all particles, rather than by simulating the millions of fluid molecules which is a lot more computationally taxing.

Now then, to the nitty gritty, what did I do for this project? Using the Brownian Dynamics simulations method, I set about creating from 250 to 750 magnetic colloidal particles with varying shifts. As they did what they pleased I set about recording several things about their interactions. Among these was the average size of the clusters they formed and the process of their nucleation. Near the end of the simulation, or when some systems reach equilibrium, I also copied data for the distribution of angles between the dipoles of bonded particles and the distribution of cluster sizes. Through doing this I could observe the dynamics of the system's growth and quantitatively study the structures formed therein.

To conclusively show these findings, I made HUNDREDS of graphs, with over some 1000 revisions in total, but due to the format and the shortness requirement I will be condensing my conclusions quite a bit. The results of all this work showed that the shift of the dipole has a meaningful impact on the size and shape of the clusters formed, and on the nature of the system itself. For systems of shift close to 0, particles tend to aggregate as chains or large looping structures. These systems can grow until all particles are part of a single cluster, hence their growth depends on the amount of particles present. As the shift of the dipole grows to 0.2 and beyond, clusters compact into ringlike structures with the dipoles towards the center, limiting further growth and causing the size of clusters to be independent of the amount of particles present.

It feels rather strange to summarize so much work in such in such few words. I've learned a LOT over the course of this project, going from not understanding any of the code I work with to improving and optimizing code of my own creation; from not having a clue what the title of my work meant, to explaining it to others. It has been trying, and fulfilling, and infuriating, and fun, and I'm glad I stuck to it. This project has helped me learn a lot about scientific research and about myself, about where my interests lie and what my goals will be. Its been a long winding road, and I am better for it.

Tags:

- Materials Science [3]

Links

[1] https://www.cienciapr.org/en/blogs/soft-matter/long-and-winding-road?language=es [2] https://www.cienciapr.org/en/user/gabrielvega?language=es [3] https://www.cienciapr.org/en/tags/materials-science?language=es