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コロイド結晶形成シミュレーションにおけるポテンシャルの影響

Potential Influence on Simulation of Colloidal Crystal Formation

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1. Introduction

Several models related to colloidal crystals formation exist, for example, DLVO potential, Sogami potential[1)], depletion force, impurity influence, and so on. To understand the mechanisms of colloidal crystals formation, a microgravity experiment was planned to suppress particle sedimentation. In the experiment plan, confocal fluorescence microscopy is a candidate of main diagnostics. Therefore, we investigated whether three dimensional coordinates of particles can be obtained by use of the microscope.

The sample conditions, that is, particle diameters, surface density of charge, and volume fraction of particles, should be decided so that which model being correct could be clarified. To determine the sample conditions, we carried out Monte Carlo simulation and summarize results as phase diagrams. The diagram based on the DLVO potential and that based on the Sogami potential are compared to find the condition causing phase difference.

2. Microscopic Observation Results

In the observation experiments, we used fluorescent polystyrene particles since the density is close to that of water. The prepared samples are shown in **Figure 1**. The colloidal sample was provided from the Yamanaka Lab. and was packed in soft bags at JAXA. The sample was observed by use of a confocal fluorescence microscope, which is basically the same model as the microscope on orbit (COSMIC). The typical observation result with void is shown in **Figure 2**. The figure clearly shows the void and particles. The void is a region without particles. To form the void, attractive force should exist.

The particle coordinates can be obtained by vertical scanning. The pair distribution function is calculated from the three dimensional coordinates. Important parameters such as the nearest neighbor inter-particle distance, and phase are obtained from the pair distribution function.

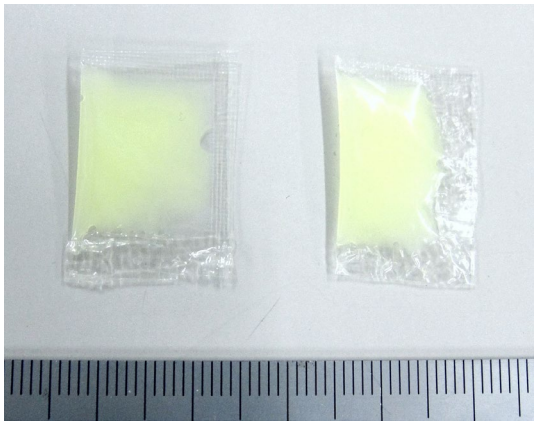


Figure 1. Fluorescent polystyrene colloidal sample bags. The colloidal sample was provided by the Yamanaka Lab. The sample was packed in soft bags at JAXA.

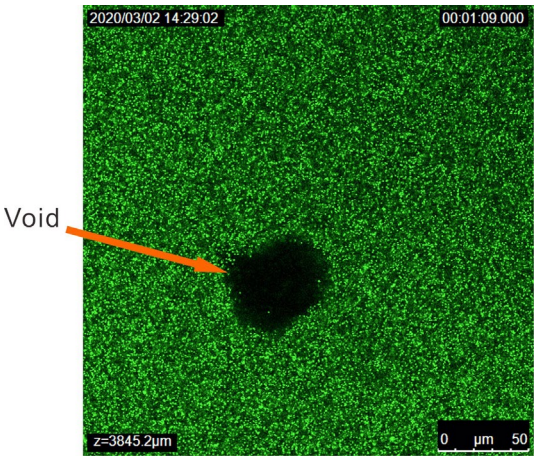


Figure 2. Typical observation result of void. Void is a region without particles. Void is clearly observed by a confocal fluorescence microscope.

3. Monte Carlo Simulation

To obtain phase diagrams in different potentials, Monte Carlo simulation is executed. A metropolis method is used in this simulation. The metropolis method is described as

$$\langle A \rangle = \frac{1}{Z}\int d\boldsymbol{r}\, A(\mathbf{r},\mathbf{p}) \exp\left\{-\frac{H(\mathbf{r},\mathbf{p})}{k_B T}\right\} \simeq \frac{1}{Z}\sum_i^N A(\mathbf{r}_i,\mathbf{p}_i) \exp\left\{-\frac{H(\mathbf{r}_i,\mathbf{p}_i)}{k_B T}\right\}, \tag{1}$$

where A, Z, H, $\mathbf{r}$, $\mathbf{p}$ are targeting physical quantity, a partition function, the Hamiltonian, coordinates, and momentum, respectively.

The typical result of pair distribution function is shown in **Figure 3**. In this case, the DLVO potential as shown in Eq. (2) is used.

$$\phi_{DLVO}(r) = \frac{Q_1 Q_2}{4\pi\epsilon_r\epsilon_0}\left\{\frac{\exp(\kappa a)}{1+\kappa a}\right\}^2 \frac{\exp(-\kappa r)}{r} + \phi_{vdW}, \tag{2}$$

where κ, Q_1, Q_2, a, ϕ_{vdW} are the reciprocal of Debye length, charge of a particle, charge of another particle, a particle diameter, van der Waals potential, respectively.

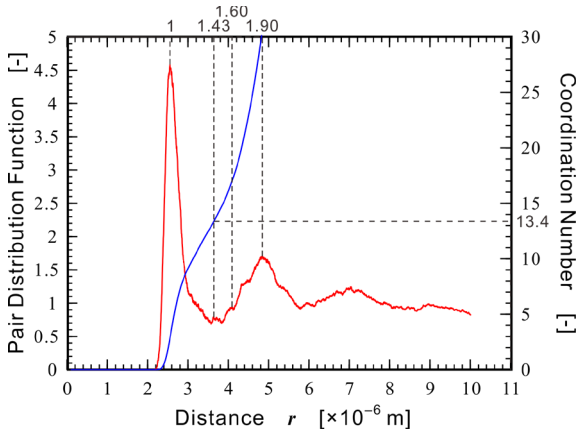
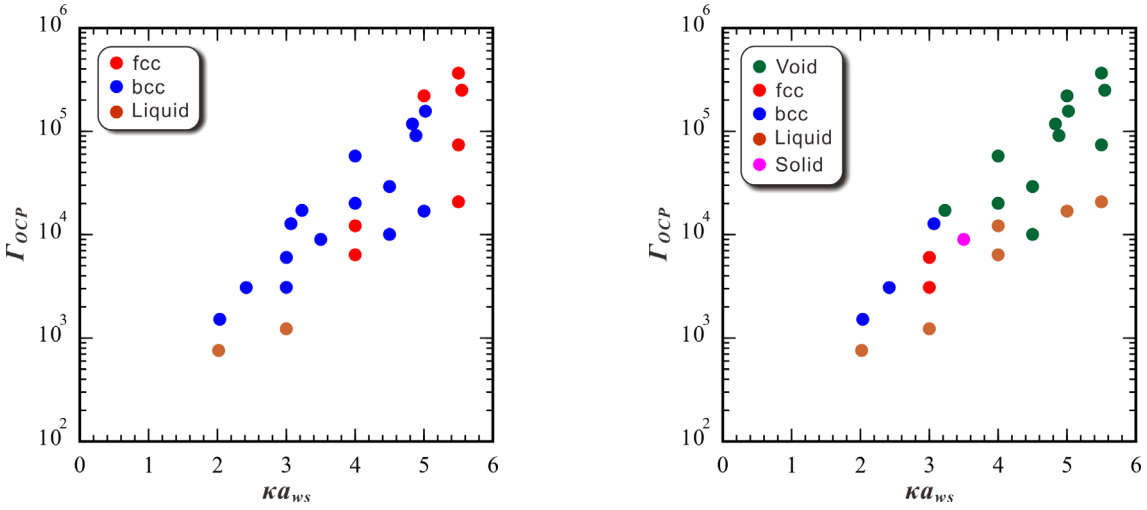


Figure 3. Typical pair distribution function calculated from simulation result. The DLVO potential is used in this case. In this calculation, the conditions of charge density of 1×10^{-7} c/cm^2, volume fraction of 1.262 vol%, particle diameter of 700 nm are used.

It is found that the structure of colloidal crystal represented in **Figure 3** is bcc, but the peak and bottom positions, and coordination number slightly differ from those of ideal values. This means the lattice is distorted. From the simulation results under various conditions, the phase diagrams are obtained.

4. Phase Diagram

Phase diagrams in cases of the DLVO and Sogami potentials are shown in **Figure 4**. In those phase diagrams, the horizontal axis is the reciprocal of Debye length multiplied by Wigner-Seitz radius, κa_{ws}, and the vertical one is the Coulomb coupling parameter, Γ_{OCP}. These parameters are generally used in complex plasmas and are usable to the colloidal suspension due to the similar system. By comparing the diagram in DLVO potential with that in Sogami potential, the particle conditions for clarifying the potential acting in colloidal suspension are determined.



(a) DLVO Potential (b) Sogami Potential

Figure 4. Phase diagrams in cases of (a) DLVO and (b) Sogami potentials. The phases represent by different colored closed circles. There is no void region in the case of DLVO potential.

5. Conclusions

It is found that the void is clearly observed, and particle coordinates are obtained by using the confocal fluorescence microscope. The coordinates are used for calculating the pair distribution function, which is used

to obtain the nearest neighbor inter-particle distance and crystal structure. To obtain the phase diagrams to determine the particle conditions for observation experiments, the Monte Carlo simulation is executed. By comparing the diagram in the DLVO potential with that in the Sogami potential, the region, in which the different phase appears in each potential, is clarified. This is useful for determination of particle conditions for observation experiments.

References

1) I. Sogami: Effective Potential between Charged Spherical Particles in Dilute Suspension, Phys. Lett., **96A** (1983) 199, DOI: https://doi.org/10.1016/0375-9601(83)90704-1.