The Effects of Confinement on Two Dimensional Jamming

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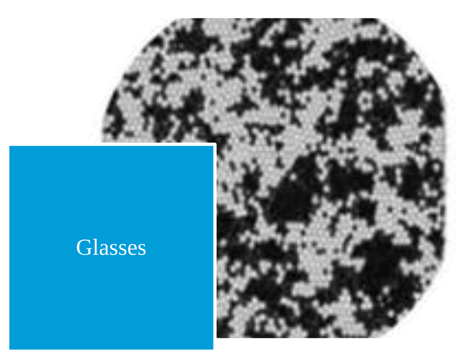
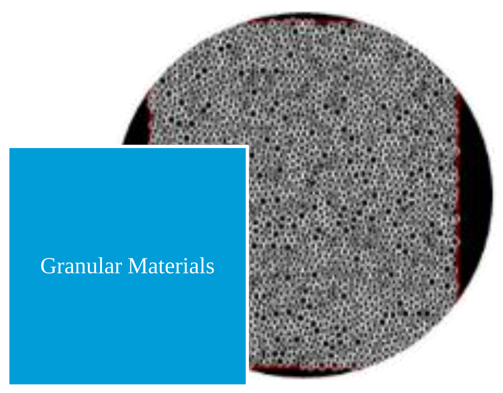
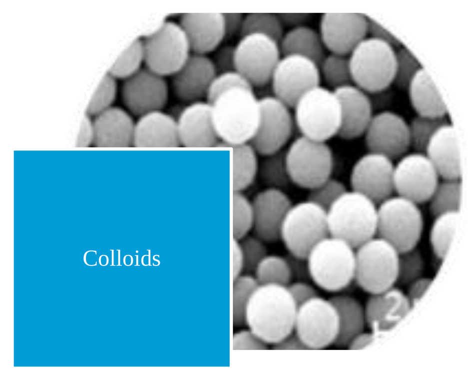
Introduction

Objective of materials research is to gain control/understanding of materials such as:





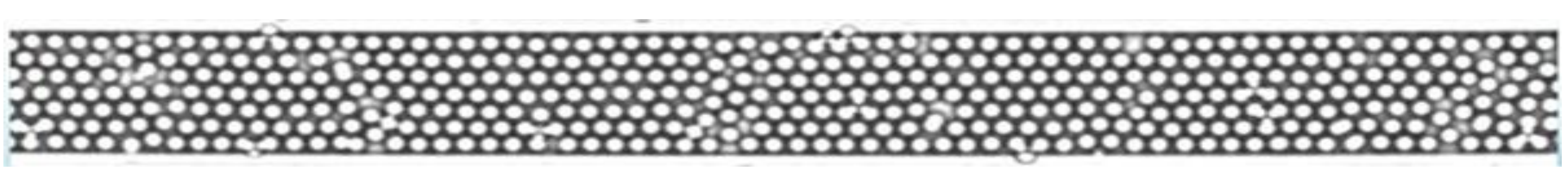


Jammed Phase – non equilibrium phase in which particles cannot move without breaking non overlap conditions

Our Objective

- ❖ Image of packed colloids or hard disks confined between two glass plates in a channel taken in the Rice lab
- ❖ Want to understand how and when the jammed phase occurs with confined systems like this in two dimensions
- ❖ Use computer simulations to achieve this goal

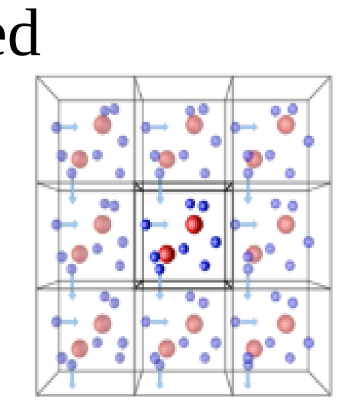
System we want to model: Hard disks con fined to a long, but narrow channel



Model

Use a **molecular dynamics simulation** with a Lubachevsky-Stillinger algorithm.

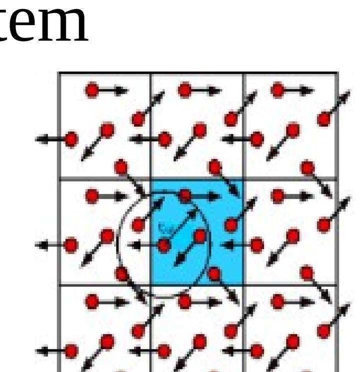
- ❖ Use disks that start as points and grow until jammed
- ❖ Track trajectories and solve equations of motion
- ❖ **Packing fraction** data collected
- ❖ **Boundary conditions** to simulate the confinement shown in the channel



Periodic Boundary Conditions (PBC)– Allows disks to re enter simulation box after leaving. Simulates an infinite system that is very long.

Hard Wall Conditions (HWC) – Disks bounce off simulation wall.

Simulations a confined box. Representative of narrow vertical confinement of the channel.



Results

Methods used to understand the data → Allow us to determine phase and when system becomes jammed

Analysis of statistical functions

- ❖ pair correlation function $g(r)$
- ❖ bond orientational function $g_6(r)$
- ❖ structure factor $S(k)$

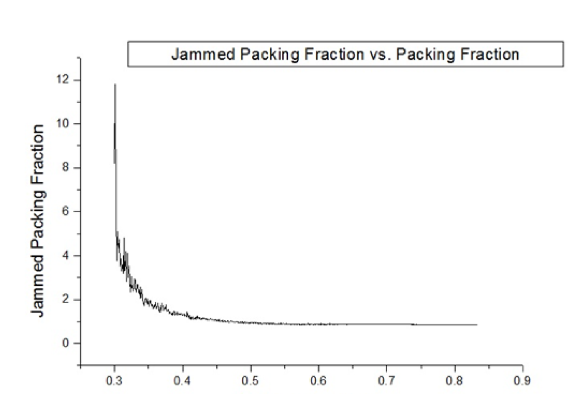
Analysis of Thermodynamic properties

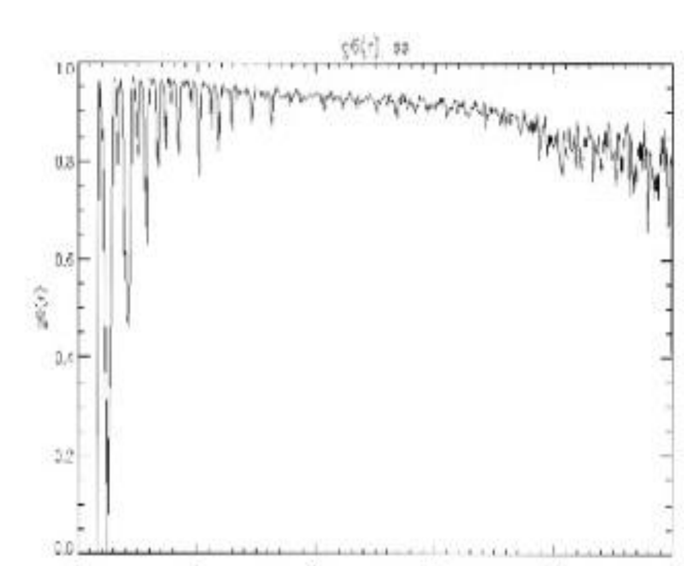
- ❖ Compressibility $Z = PV/Nk_BT$
- ❖ packing fraction ϕ

What to look for in these functions to determine a jammed state:

1. A decay rate of $\frac{1}{r^3}$ in $g(r)$. Closer fit indicates presence of long range order
2. Decay to a nonzero value in $g_6(r)$
3. Asymptotic behavior of Z
4. A packing fraction around 0.84 (density)

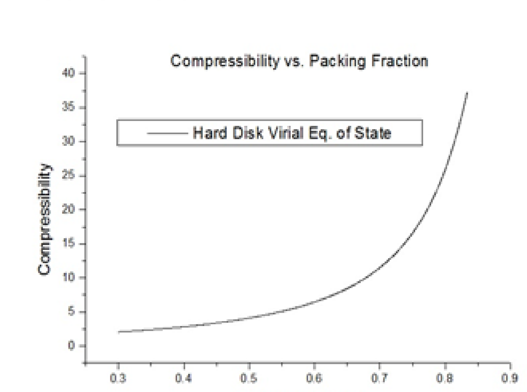
Many other criteria are also required, however, our study is focused on these points.

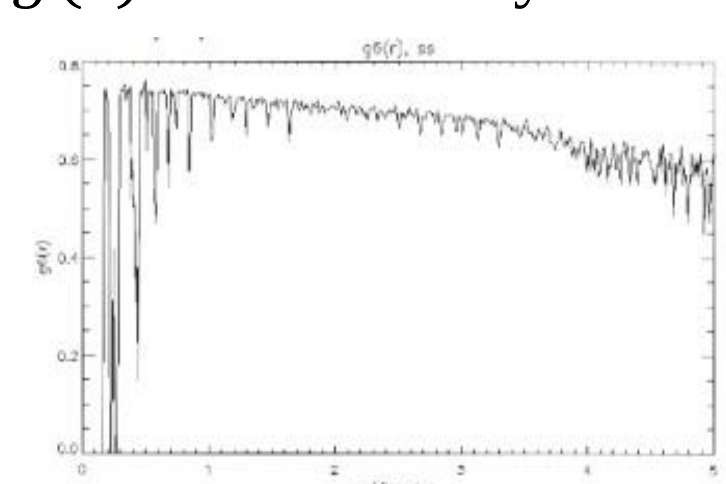




$g(r)$ exhibits decay rate of $\frac{1}{r^3}$

Estimated of jammed ϕ is 0.84
Z becomes asymptotic as the jammed ϕ is reached





$g_6(r)$decays to nonzero value

Conclusions

- ❖ Jammed ϕ occurred around 0.84. Consistent with literature
- ❖ Disks grown in all PBC (totally infinite system) and with PBC in one dimension and HWC in one dimension (modeled a channel). In the latter, ϕ = 0.84 had more solid-like properties, so the $g(r)$ showed a decay rate of $\frac{1}{r^3}$ and $g_6(r)$ stronger decay to a nonzero value
- ❖ Significance of this finding is that **confinement has a direct effect on lowering the packing fraction at which the system reaches solid-like or jammed-like properties**

Literature Cited

[1] A. H. Marcus, J. Schofield, S. A. Rice, Phys. Rev. E: Stat. Phys., Plasmas, Fluids, Relat. Interdiscip. Top. 1999, 60, 5725-5736.

[2] M. Skoge, A. Donev, F. H. Stillinger, S. Torquato, Phys. Rev. E: Stat., Nonlinear, Soft Matter Phys. 2006, 74, 041127/041121-041127/041111.

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