Monte Carlo Simulations of Dense Particle Packings: Applications to Material Self-Assembly and Batteries

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Background

Packing theory is crucial for creating efficient interfaces in a solid-state battery, to not inhibit the charge mobility. By packing densely, charges are more likely to contact with the electrolyte and undergo a redox reaction to cause a current.

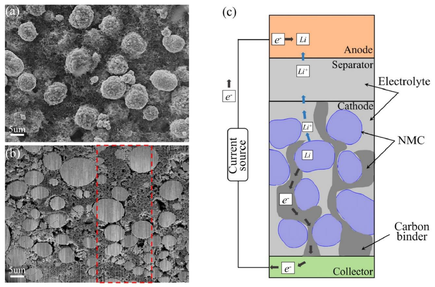

Figure 1: A top and side view of the interface's microstructure is shown in (a) and (b). A side view of the solid-state battery cell is shown in (c). The path of a lithium charge as it discharges an e- is depicted. [1]

Methodology

To emulate random particle movement and space deformation, Monte Carlo (MC) method is utilized. The code runs in stages, with each stage having 2 steps.

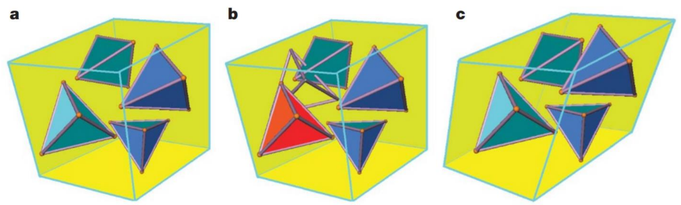

Figure 2: The steps for the MC simulation is displayed in 1a, 1b, and 1c. [2]

Results

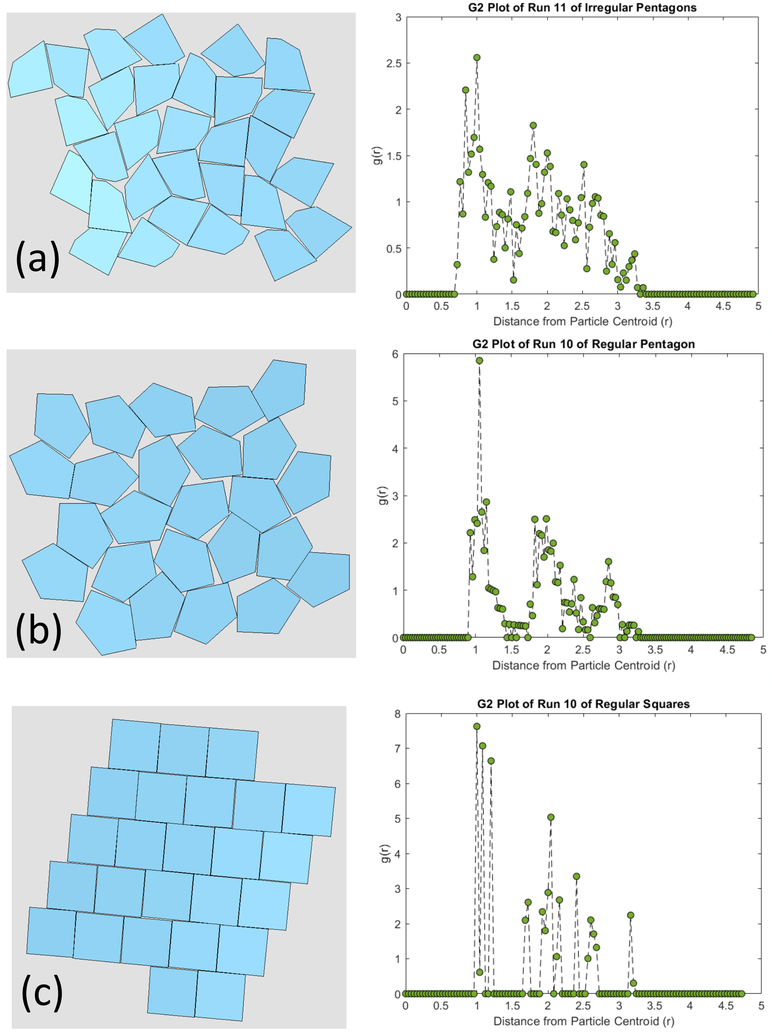

Figure 3: Packings and g(r) graphs shown of (a) Irregular pentagon, (b) regular pentagon, and (c) regular square.

Discussion

Figures 3a, 3b, and 3c feature a visualization and the g(r) graph for the system. These two images show certain trends in the different test cases which can also apply to a real, crystal system.

1.) As shown in figure 1a and 1b, as regularity increases so does packing. Crystallinity increases.

2.) Packing is dependent on the symmetry of the particle. Ordered packings occurs if local symmetry aligns with global symmetry, with ordered packings implying crystallinity.

3.) The g(r) function quantifies the state of order within the system, with higher values indicating higher packing. The function is also used to determine deviation from unity.

Application

Solid-state batteries have not achieved conductivity comparable to lithium-ion batteries. Sintering has been used to improve these batteries to pack tiny particles closer, and manipulation of sintered particles can engineer a better thin-film interface. And if the particle is optimal enough, self-assembling interface is possible.

[1] R. Xu, Y. Yang, F. Yin, P. Liu, P. Cloetens, Y. Liu, F. Lin and K. Zhao, Journal Of The Mechanics And Physics Of Solids 129, (2019).
[2] S. Torquato and Y. Jiao, Nature 460, (2009).

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