HOPPING THROUGH THE INTERFACES: A MULTISCALE CHEMO-MECHANICS MODEL FOR SOLID-STATE BATTERY ENERGY MATERIALS

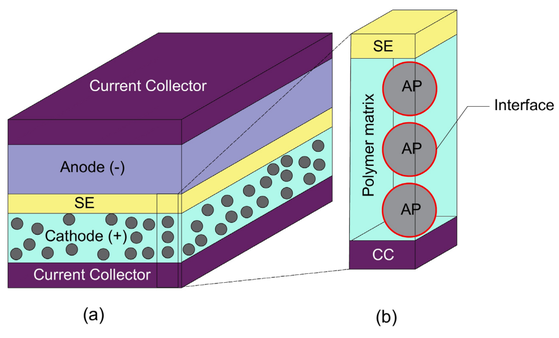
Towards a Digital Twin of Cathode Microstructure

Jacqueline Lee; Supervisors: Sehoil Bazazzadeh[1], Łukasz, Figel[1]

1. International Institute for Nanocomposites Manufacturing (IINM), WMG, University of Warwick, Coventry, CV4 7AL, UK

Introduction

ABAQUS is a software that can simulate diffusion mechanics for lithium-ion batteries (LIBs). However, drawing 3d shapes manually to model cathode and active particles (APs) in the software is inefficient.

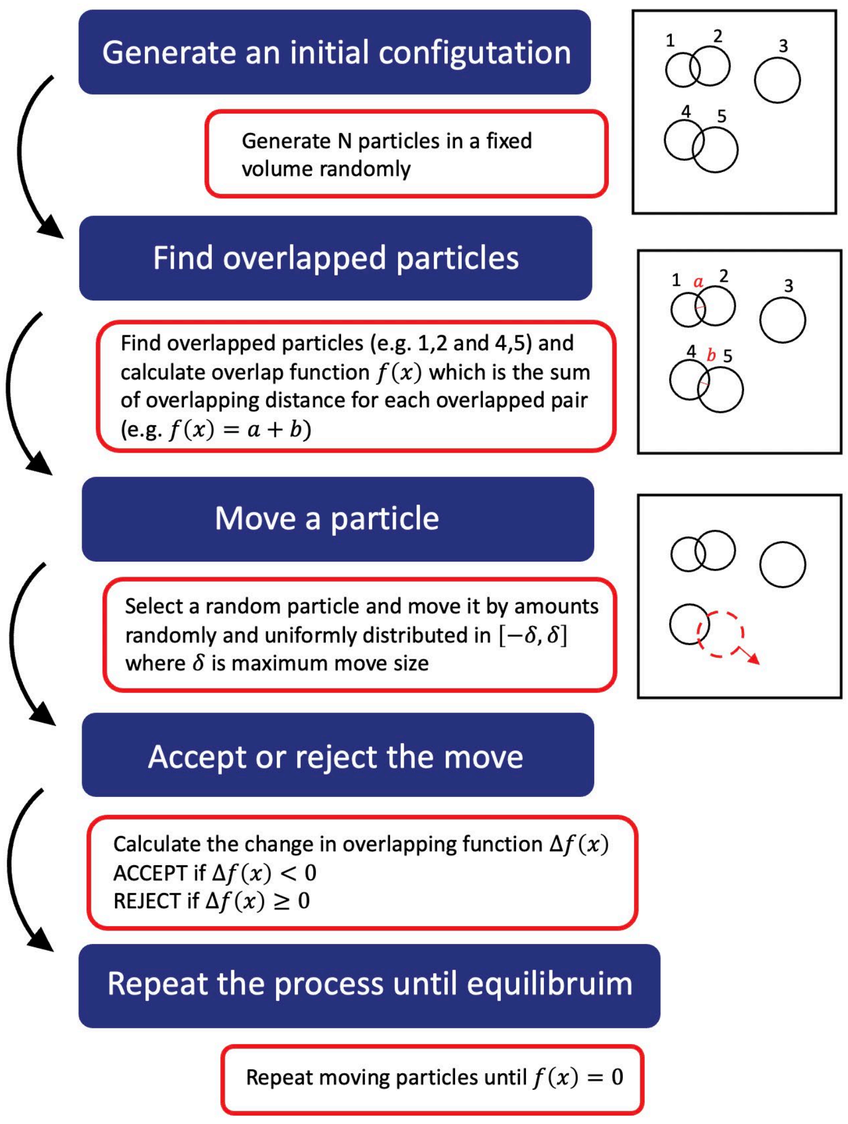


(a) (b)

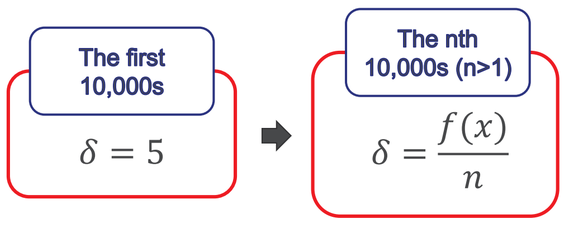
- **Aim:**
  Find an arrangement for APs in the cathode with an algorithm and achieve the volume fraction as high as possible.

Methods

- Assumptions: APs are considered as idealised spherical shapes
- Build an algorithm to find an optimal arrangement for spheres (APs) in a box (cathode)



- The importance of choosing δ: A large value might cause most steps to be rejected whereas a small value might make the system evolve slowly.
- δ exploration:
  The maximum step size δ changes in every 10,000 iterations.



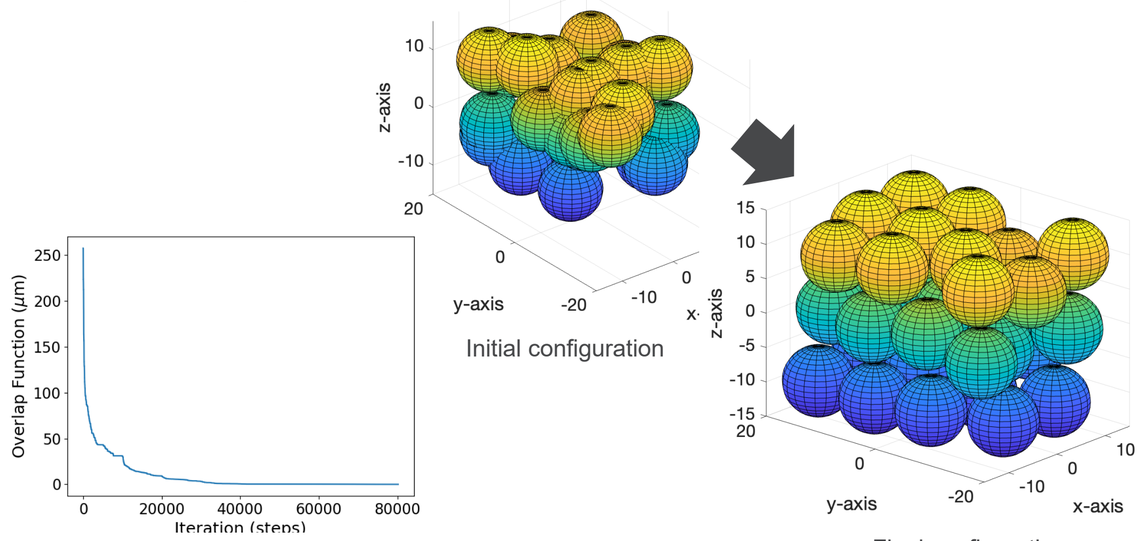
*$f(x)$ = overlap function
n = the number of ball pairs overlapped

Results

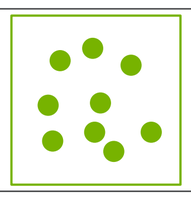
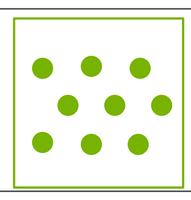
1. APs with same size

Parameters:
- Size of cathode = 30×40×30 (μm^3)
- Radius of APs = 5 (μm)
- The minimum distance between two APs = 0.15 (μm)

- The overlap function decreases as particles move around and reaches to zero eventually



- Torquato, S. [1] suggested that starting with a hexagonal arrangement may be more efficient than a random arrangement to attain high densities
- Two possible initial configurations:

	Random Arrangement	Hexagonal Arrangement
Maximum Archieved Volume Fraction	0.465 (32 balls)	0.451 (31 balls)
Excuate Time (s)	76	41
Figure		

- To simulate high energy density cathode in ABAQUS, our desired algorithm is to achieve the volume fraction as high as possible
- Setting the initial configuration as a random arrangement may be more advantageous to used than a hexagonal arrangement

2. APs with two sizes

Parameters:
- Size of cathode = 30×40×30 (μm^3)
- Radius of APs = 3&5, 5&8 (μm)
- The minimum distance between two APs = 0.15 (μm)

- Random arrangements were chosen for generating initial configuration
- For 40 APs, the achieved maximum volume fraction is 0.456

Radius (μm)	3&5	5&8
Maximum Archieved Volume Fraction	0.456 (40 balls)	0.426 (20 balls)
Ratio	1:3	4:1
Excuate Time (s)	356	11

* The radius was selected according to the experimental observations by [3]

Conclusion

- The maximum volume fraction the algorithm can achieve is 0.465 for single size balls and 0.456 for two size balls
- Setting a random arrangement as the initial configuration is advantageous to reach a higher volume fraction

Further work

- Implement the current algorithm for different size of APs
- Improve the algorithm to achieve a higher volume fraction and decrease the execute time with the method suggested by [2]

Intern Bio

Jacqueline Lee is studying physics at Imperial College London. She is interested in solving real world engineering problems and understanding the theoretical aspects of engineering. She aspires to be a mechanical engineer or a researcher in mechanical engineering.

References

[1] Salvatore T., *Random Heterogeneous Materials.* Springer-Verlag; 2002. https://link.springer.com/book/10.1007/978-1-4757-6355-3

[2] Chen, D. Z. et al. Algorithms for congruent sphere packing and applications. *Association for Computing Machinery.* 2001: 212–221. https://doi.org/10.1145/378583.378672

[3] Shi, T. et al., High active material loading in all-solid-state battery electrode via particle size Optimization. *Advanced Energy Materials*. 2020;10(1902881). 10.1002/aenm.201902881

THE FARADAY INSTITUTION SOLBAT NEXT GENERATION SOLID-STATE BATTERIES

WARWICK THE UNIVERSITY OF WARWICK

Imperial College London

UK Research and Innovation