Simulation of Glancing Angle Deposition (GLAD)

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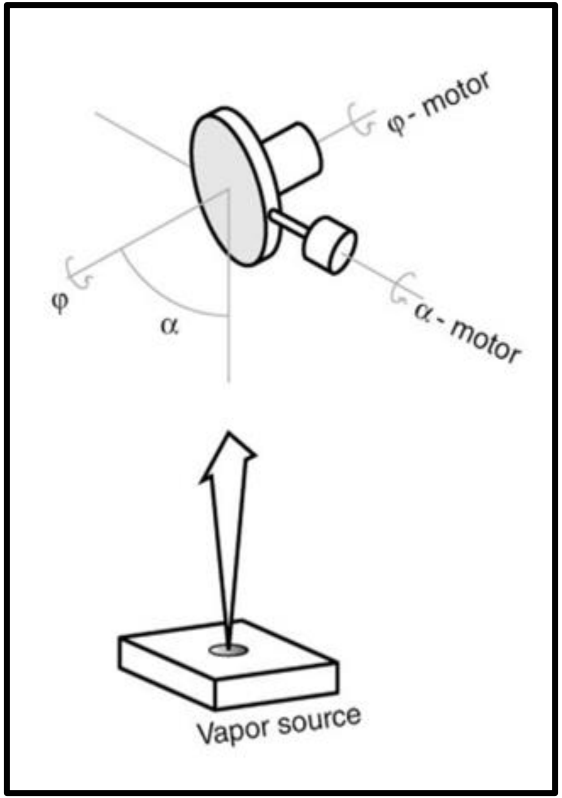
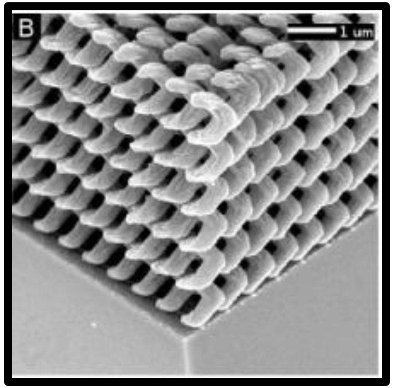
Introduction

[1]

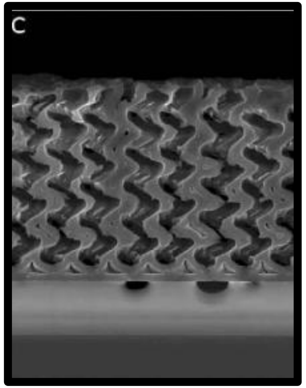


- GLAD is a bottom-up nanomanufacturing technique for thin films.
- The incident angle (α) and azimuth rotation angle (φ) are manipulated to produce shadowing which results in self-assembled nanostructures.
- Applications in sensing, optics, magnetic storage and other fields.

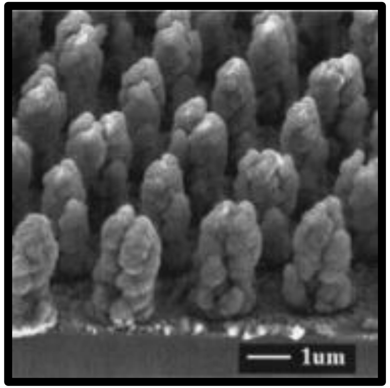
Optics [1]



Sensing [1]



Magnetic Storage [2]

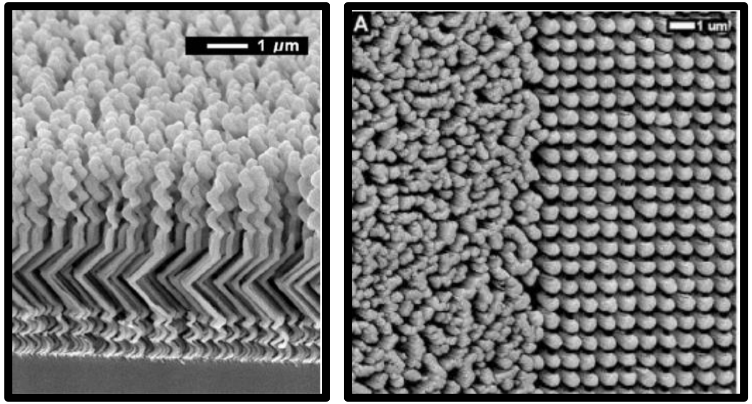


[1] M. Taschuk, M. Hawkeye, M. Brett, *Handbook of Deposition Technologies for Films and Coatings*, William Andrew Publishing, 2010. p. 624, p. 629, p. 630
[2] B. Dick, M. J. Brett, T. J. Smy, M. R. Freeman, M. Malac, and R. F. Egerton, "Periodic magnetic microstructures by glancing angle deposition," Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films, vol. 18, no. 4, pp. 1838–1844, Jul. 2000, doi: 10.1116/1.582481.

GLAD Theory and Design Elements

- Ballistic shadowing causes particle structures to grow and reduce in size.
- Different seeding patterns can be used.
- Natural seeds are cost effective but do not provide much initial control over deposition.
- Predetermined seeds are time consuming but allow for more control over nanostructures.

Natural seeding Pre-seed



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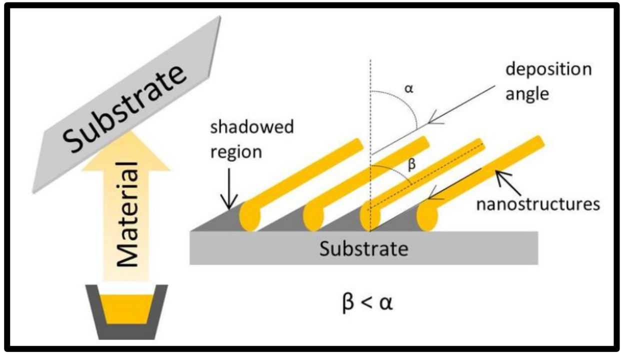


[2]

[1] M. Taschuk, M. Hawkeye, M. Brett, *Handbook of Deposition Technologies for Films and Coatings*, William Andrew Publishing, 2010. p. 634
[2] H. Chu, S. Song, C. Li, and D. Gibson, “Surface Enhanced Raman Scattering Substrates Made by Oblique Angle Deposition: Methods and Applications,” *Coatings*, vol. 7, no. 2, p. 26, Feb. 2017, doi: 10.3390/coatings7020026.

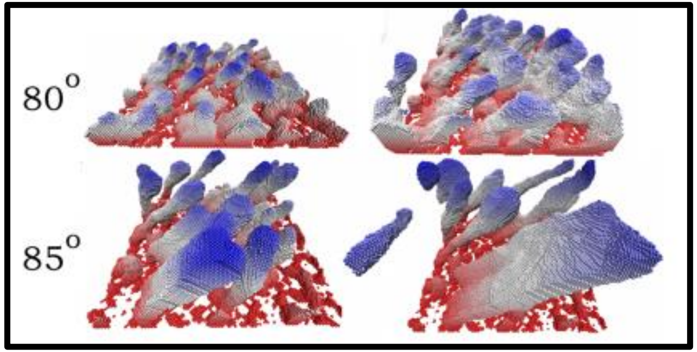
Research Project Goal

Develop a 3D simulation of the GLAD process for fabricating nano-structures which includes the following:

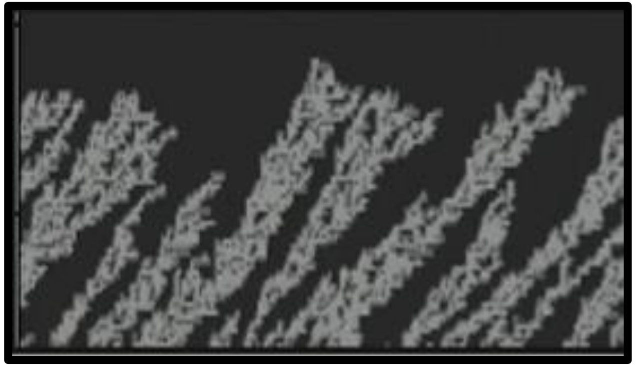
- Allow the user to modify both incidence angle (α) and azimuth rotation angle (φ).
- Allow for the prediction of various seeding strategies (both natural and pre-seeds).
- Uncover the relationship between α and column growth angle (β).

Images from: M. Taschuk, M. Hawkeye, M. Brett, *Handbook of Deposition Technologies for Films and Coatings*, William Andrew Publishing, 2010. , p. 648, p. 663

Background and Previous Research



[1]

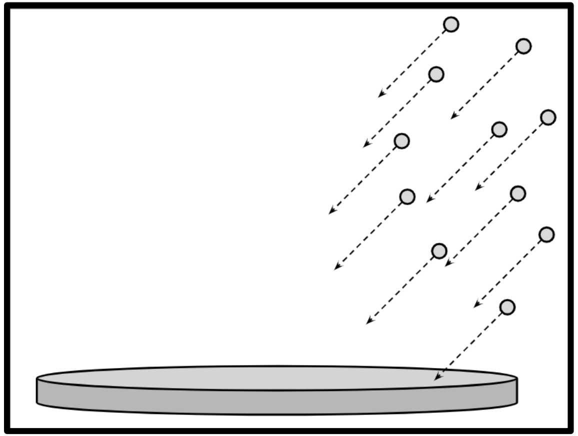


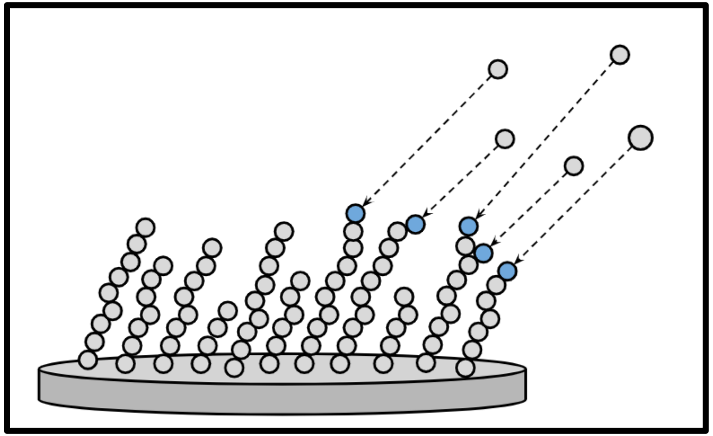
- Simulation was excessively slow and required specific hardware to run. (100+ Hours)
- 2D simulation does exist but is inaccurate on a large scale.

[1] B. C. Hubartt, X. Liu, and J. G. Amar, “Large-scale molecular dynamics simulations of glancing angle deposition,” Journal of Applied Physics, vol. 114, no. 8, p. 083517, Aug. 2013, doi: 10.1063/1.4819446.

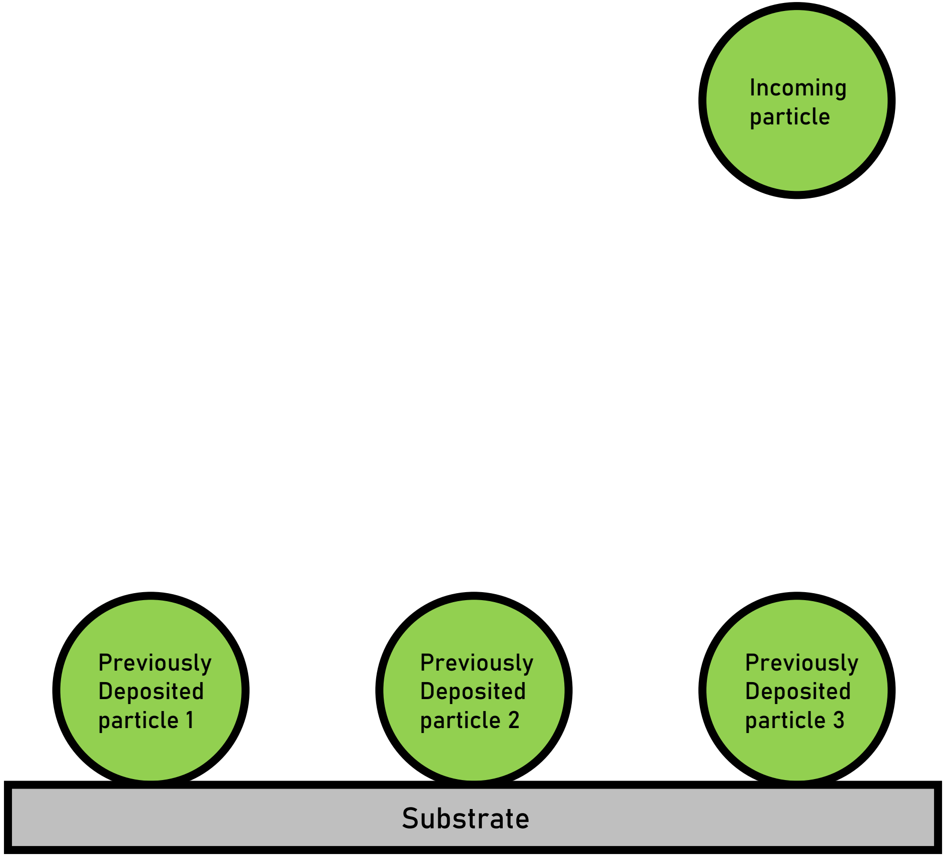
Simulation Idea

- Particles will enter scene from specific incidence angle.
- Incoming particles will check for any collisions that happen.
- Land at their appropriate positions.



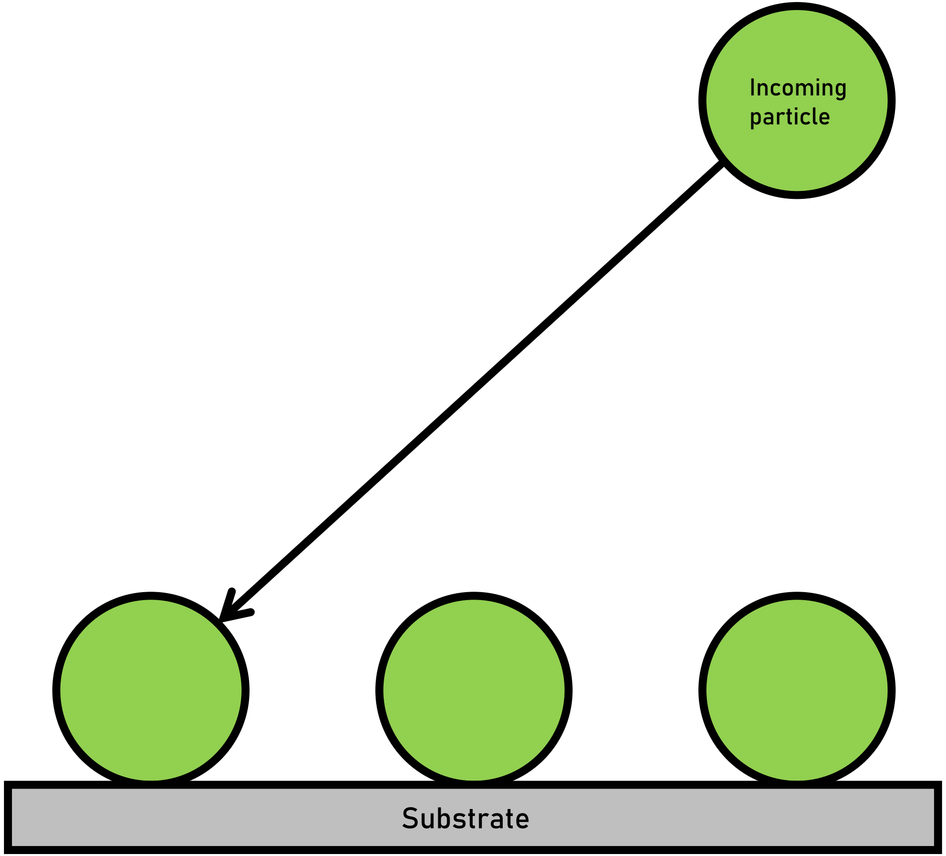


Collision Resolution Algorithm



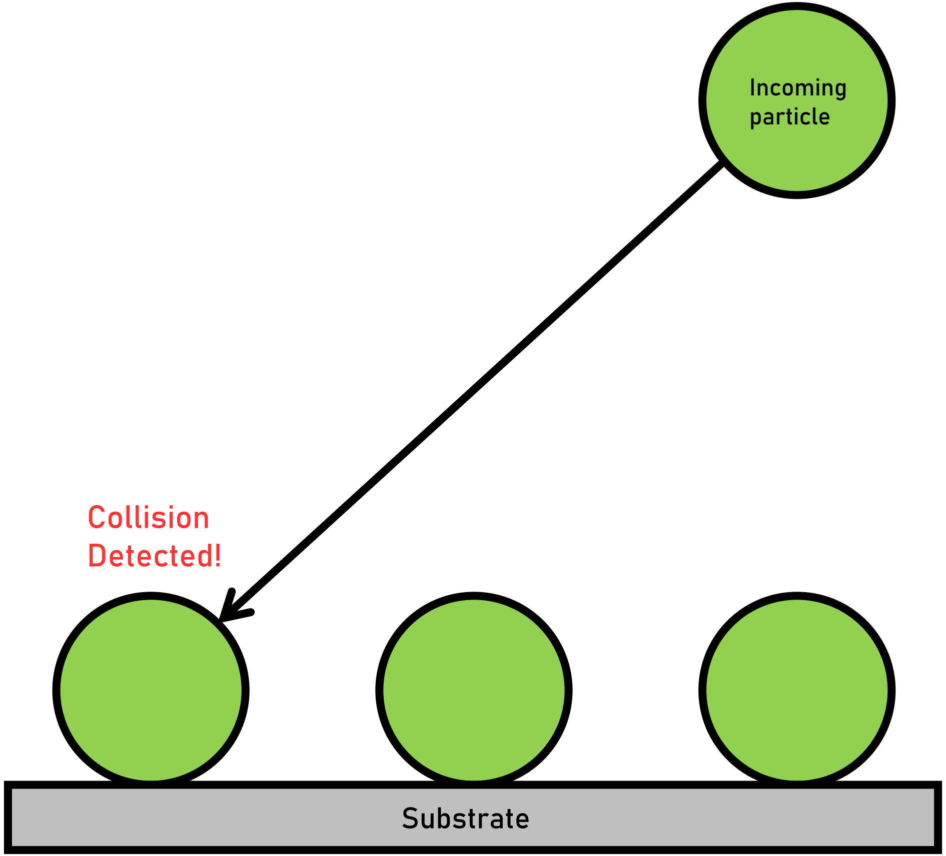
- New particle enters scene.

Collision Resolution Algorithm



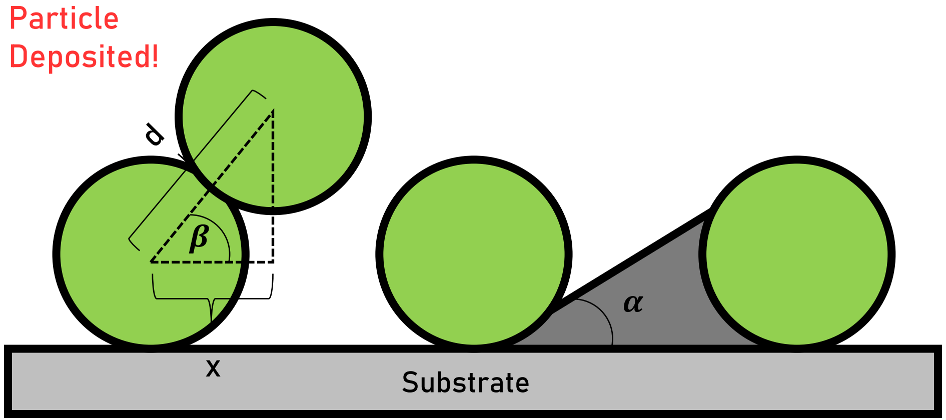
- New particle enters scene.
- Casts a vector-ray from its initial position to its destination.

Collision Resolution Algorithm



- New particle enters scene.
- Casts a vector-ray from its initial position to its destination.
- If the ray intersects anything in its path, particle will land at the intersection point.
- If it doesn't, then particle will land on substrate.

Collision Resolution Algorithm



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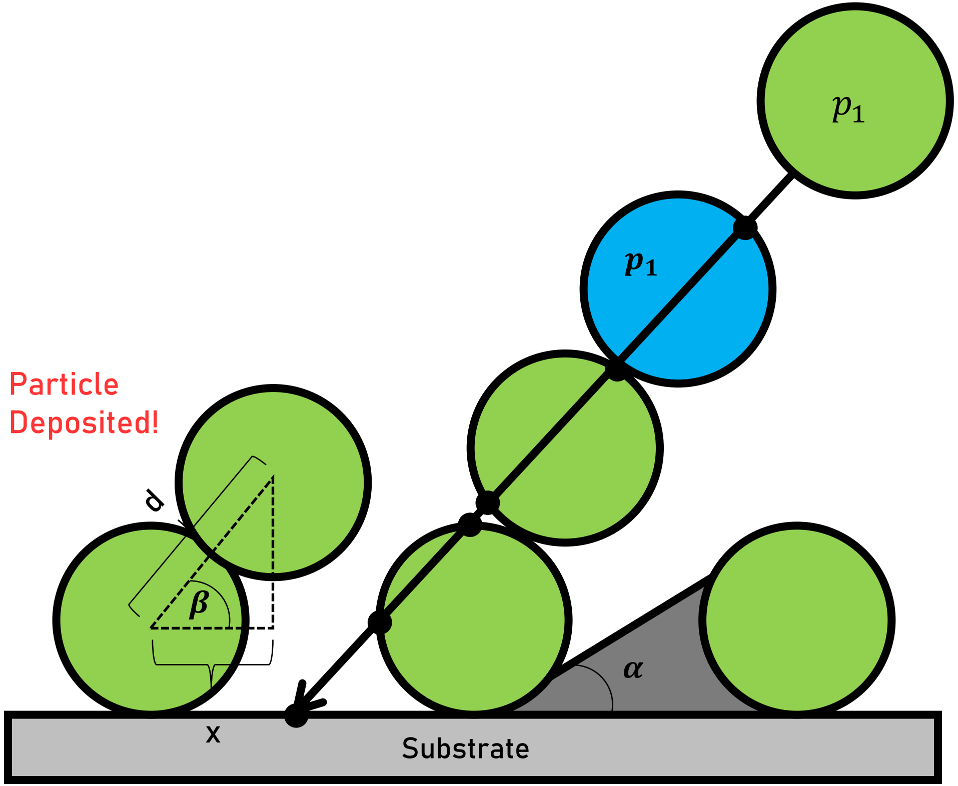
- Steps repeated until all particles (~35,000 particles) have settled to their final positions.
  - $x = d * \cos\beta$

Collision Resolution Algorithm



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Demonstration of Simulated Growth

Sphere seeds are simulated at 80^o incident angle.

Percent Coverage: 31.79 %.

Depends on the variance of the incidence angle.

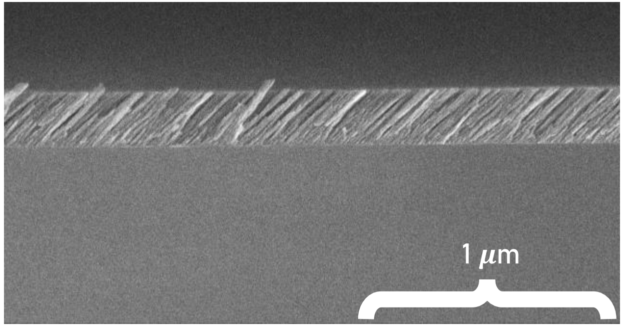
Simulation of Natural Seed Growths

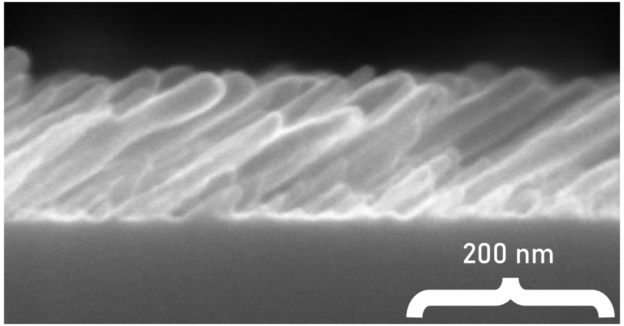
$\alpha = 75^o$

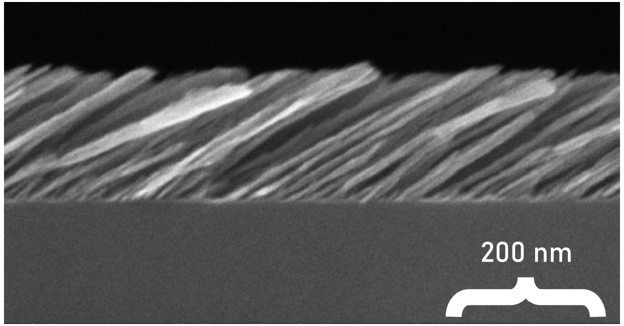
$\alpha = 80^o$

$\alpha = 85^o$

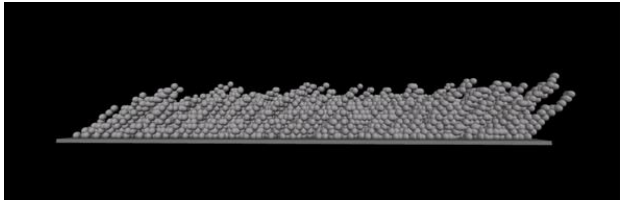
SEM Images

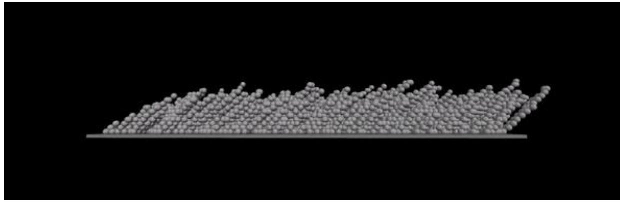


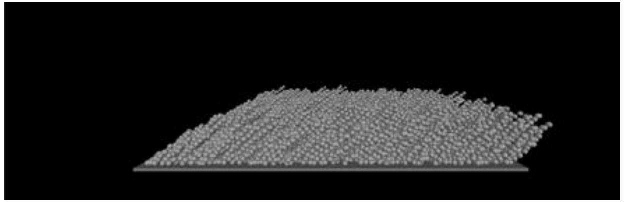


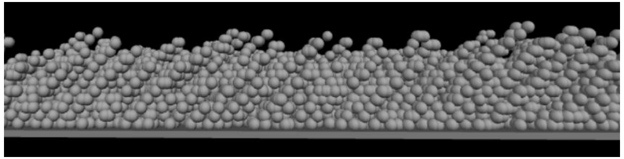


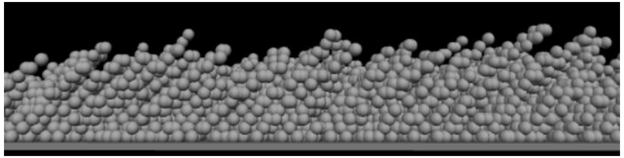
Simulated

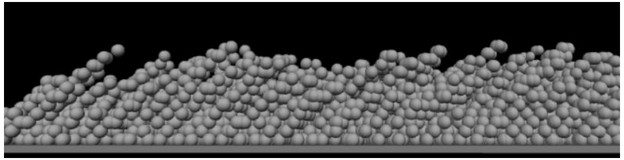












Comparison of Simulation vs. Experiment

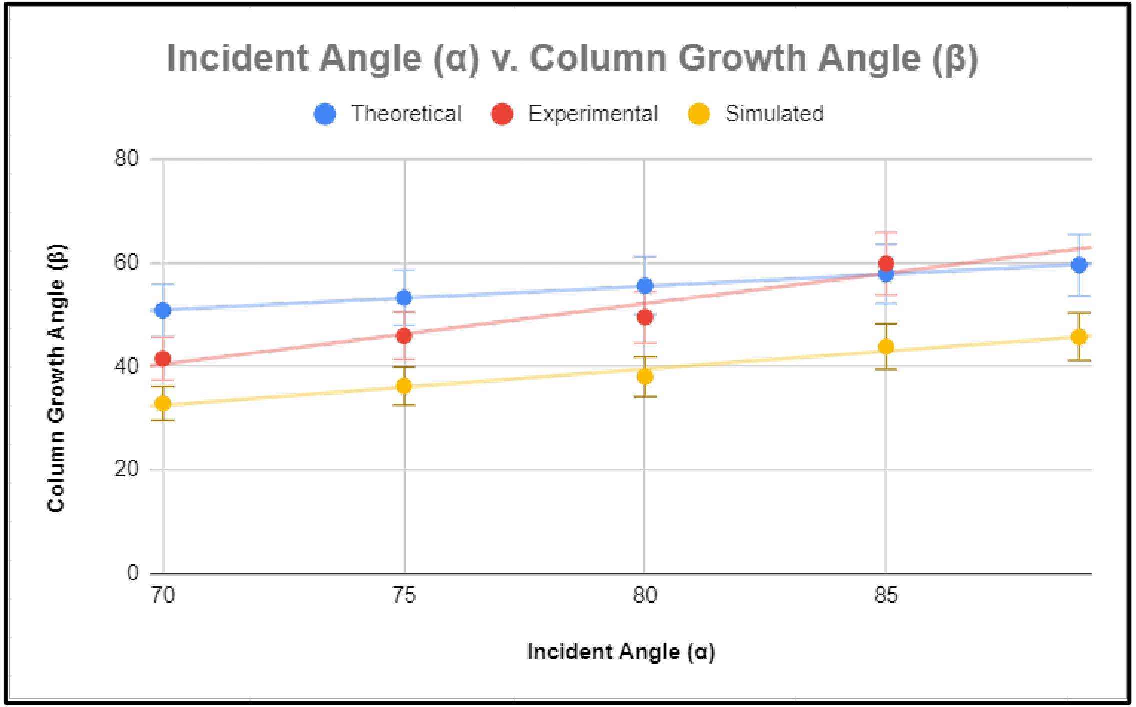
Main parameter to test is the column growth angle (β).

Demonstrated: $\beta < \alpha$

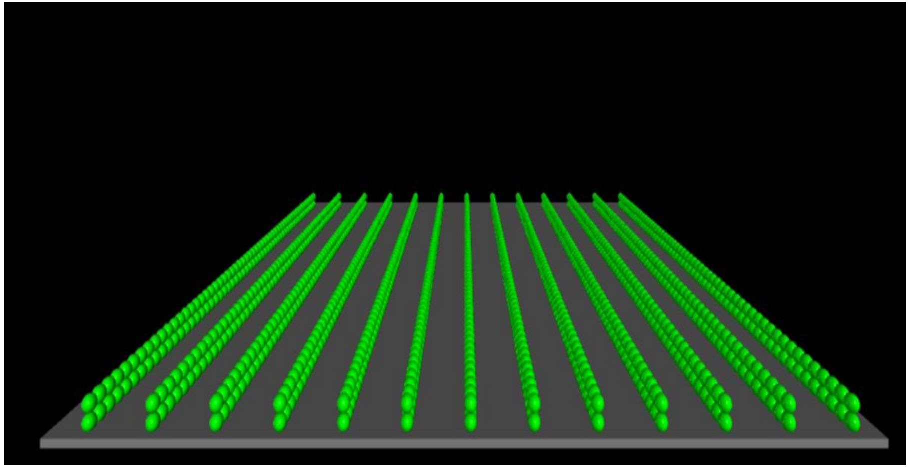
Tait's Rule (Theoretical)

$$\beta = \alpha - \sin^{-1}\left(\frac{1 - \cos(\alpha)}{2}\right)$$

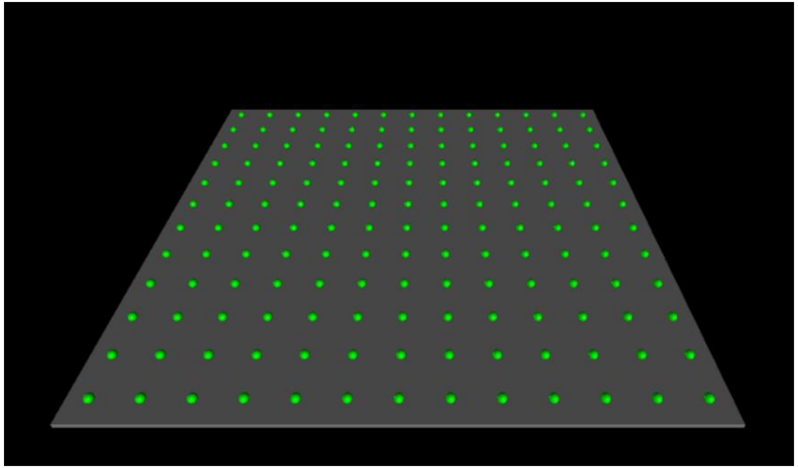
For $\alpha < 70^o$, continuous thin films are observed and thus cannot be compared.



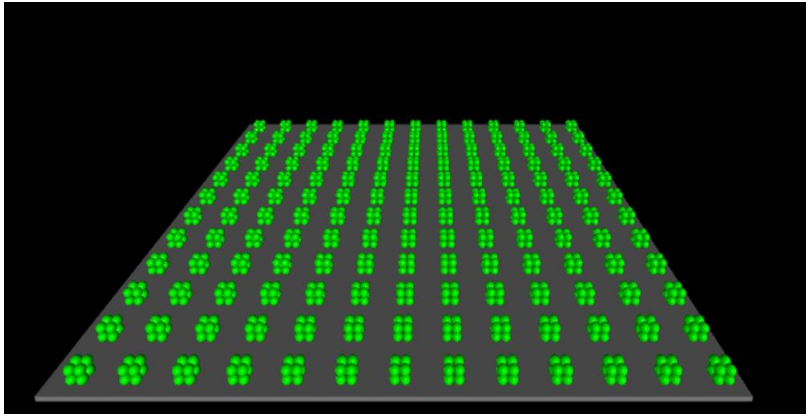
Seeding Patterns



Line Seeds

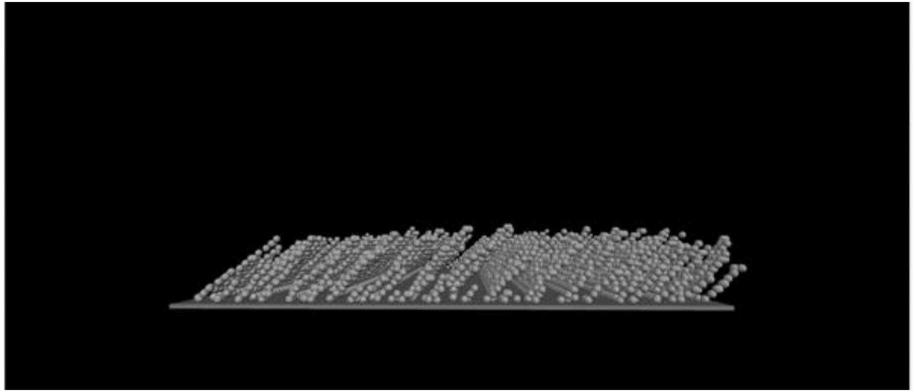


Spherical Seeds

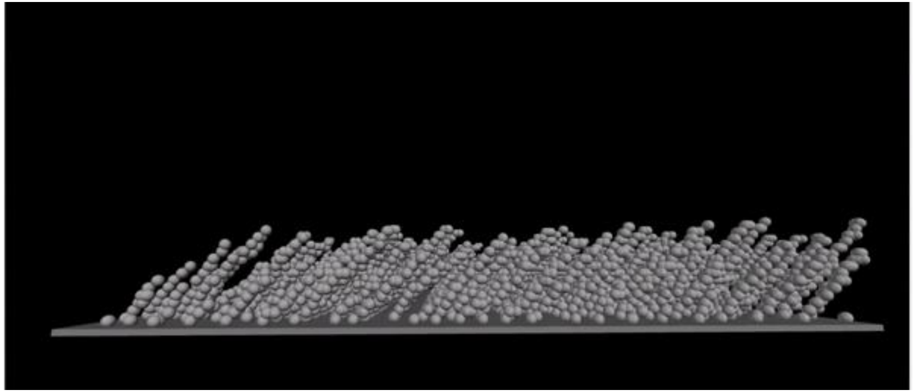


Cube Seeds
with flat tops

Simulated Growth on Pre-seeds



Line Seeds



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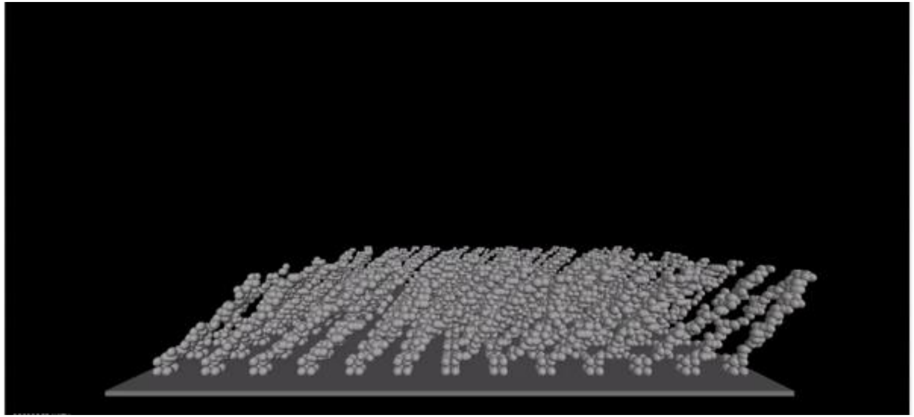
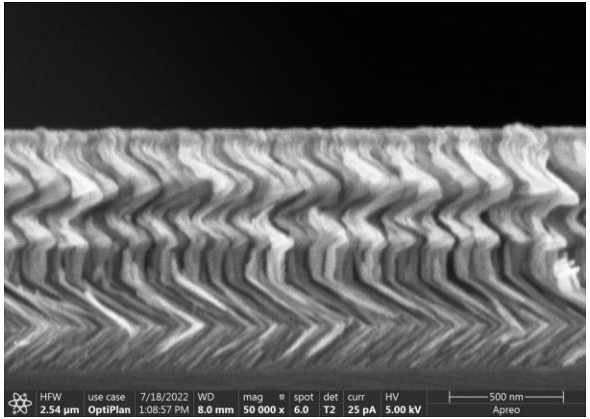
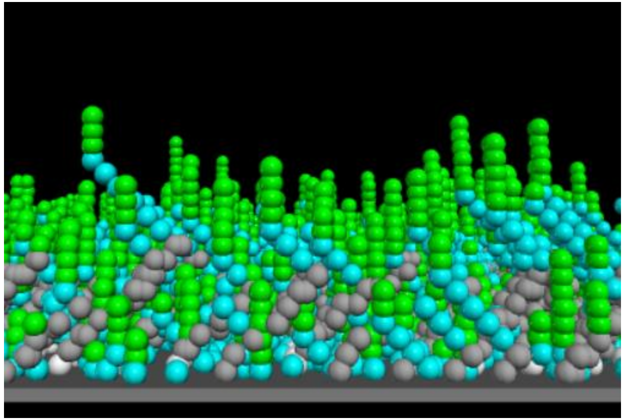


Cube Seeds with flat tops

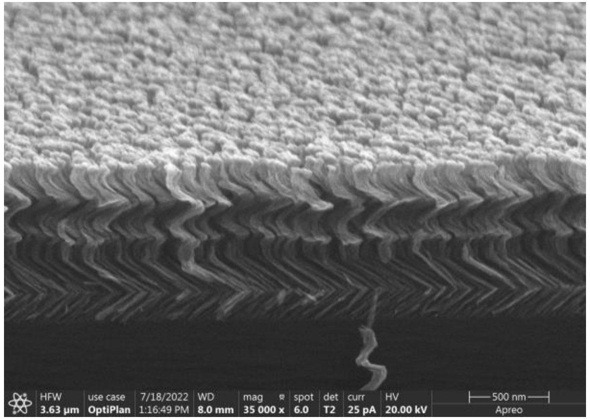
Simulated Growth of Complex Structures

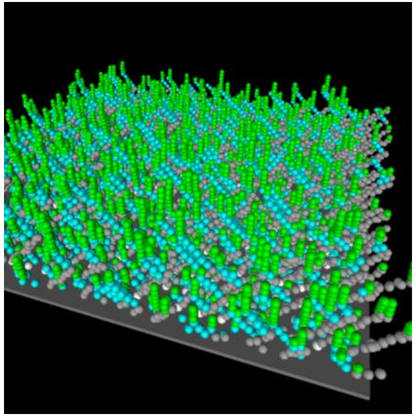


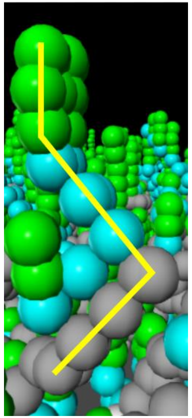


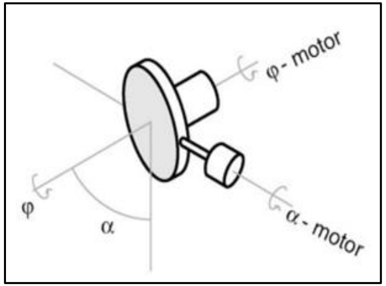
- Used a spontaneous recipe to create zigzag, rod, and helix

  •Zig-Zag: $\alpha = 75^o,\ 80^o$
  •Column: $\omega = 5\, rpm$
  •Helix: $\omega = 0.04\, rpm$









Program Efficiency

Time Complexity	Iterations	Render Time (s)
$O(n^4)$	$x < 2{,}500{,}000{,}000$	38.55
$O(n^3 + n^2)$	$x < 510{,}000{,}000$	12.36
$O(n^3 + n)$	$x < 500{,}000{,}000$	9.79
$O(sn^3)$	$x < 100{,}000{,}000$	3.54

We developed and tested 4 algorithms and the last one turned out to be the most efficient.

Conclusions

- Implemented 3D simulation of the GLAD process in a Monte-Carlo Fashion
- Demonstrated growths on natural and predetermined seeds.
- Outputs include percent coverage, and simulated column growth angle.
- Developed efficient collision resolution algorithms.

Acknowledgements

NSF

IMPACT-NG R.E.U.

Research Experience for Undergraduates

NSF Award ID #1950137

NSF Award ID #2025075

National Nanotechnology Coordinated Infrastructure

KY MULTISCALE

Thank you

Future Work

- Adding surface diffusion to landed particles
- Adding support for various deposition materials:
    - Currently only supports Germanium
- Adding support for changes in pressure