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# AN ATOMISTIC STUDY OF NANOSCALE SINTERING: APPLICATION TO ADDITIVE MANUFACTURING

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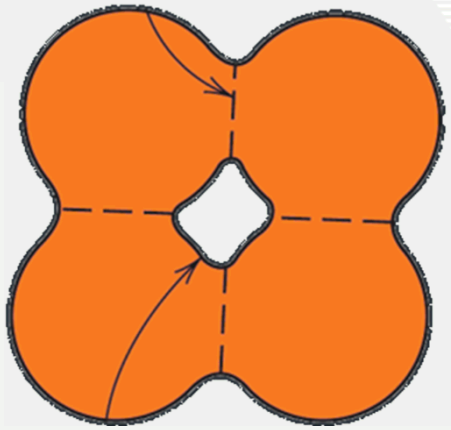
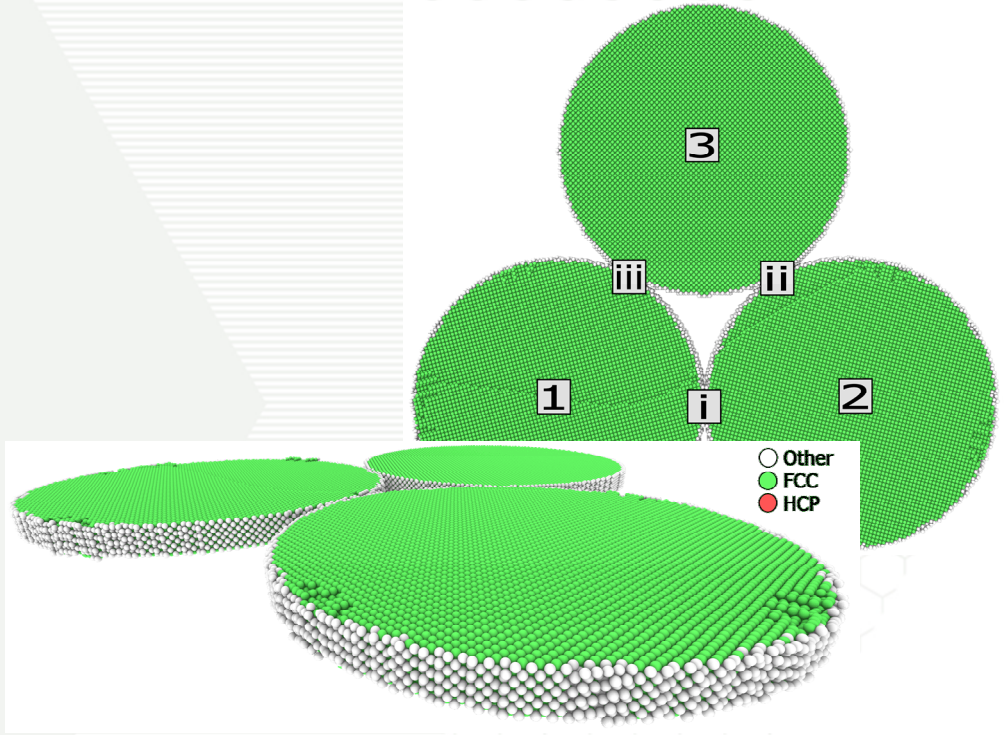
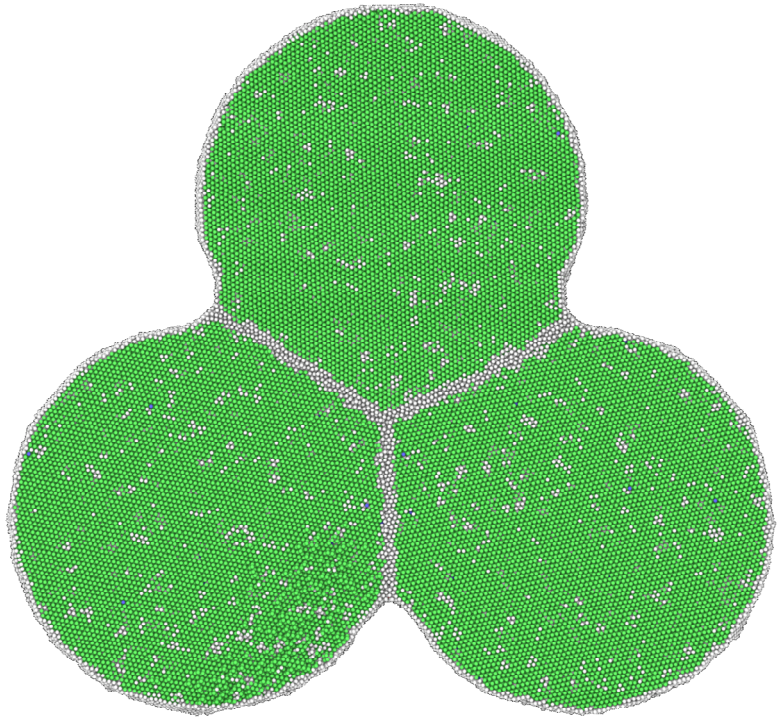
# OUTLINE



Sintering Background

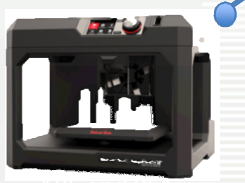



- Objective
- Model Setup

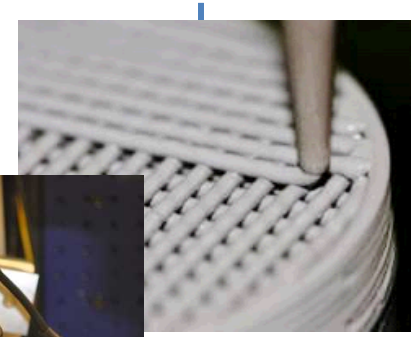


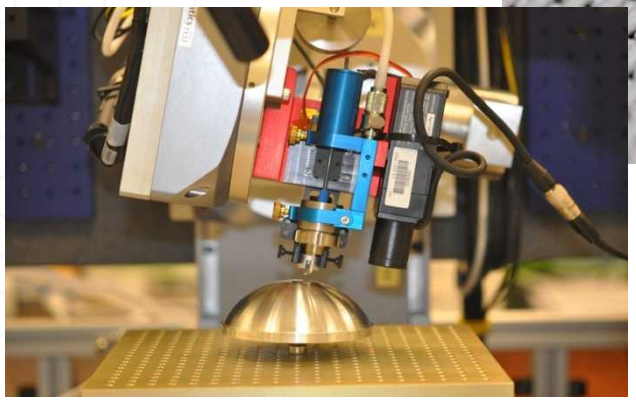
Sinter Results

# ADDITIVE MANUFACTURING



*Custom, open architecture materials research & manufacturing capabilities*



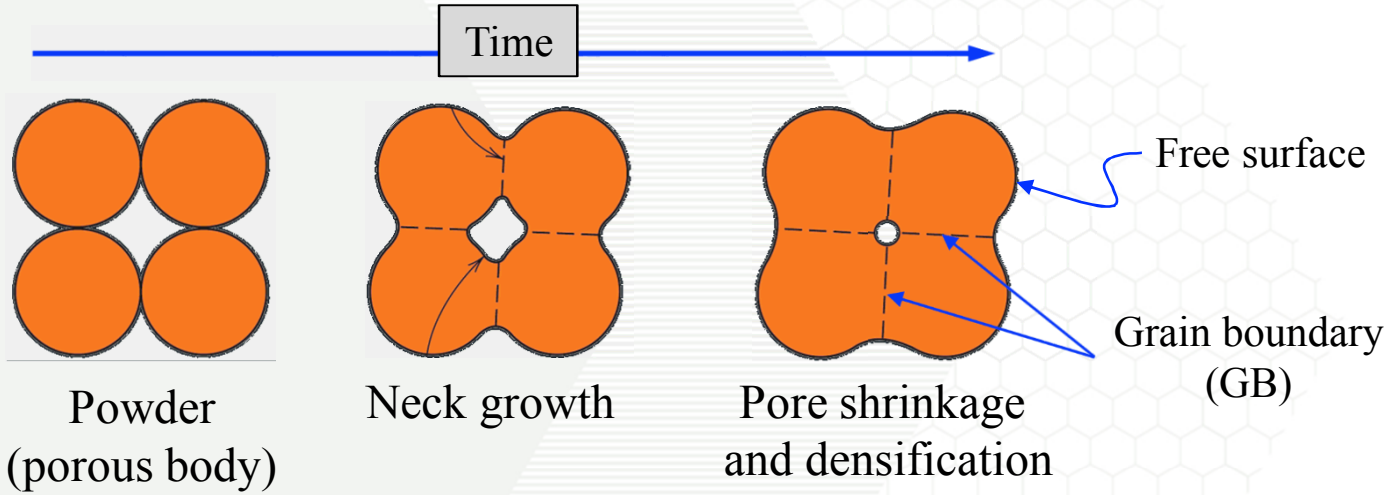


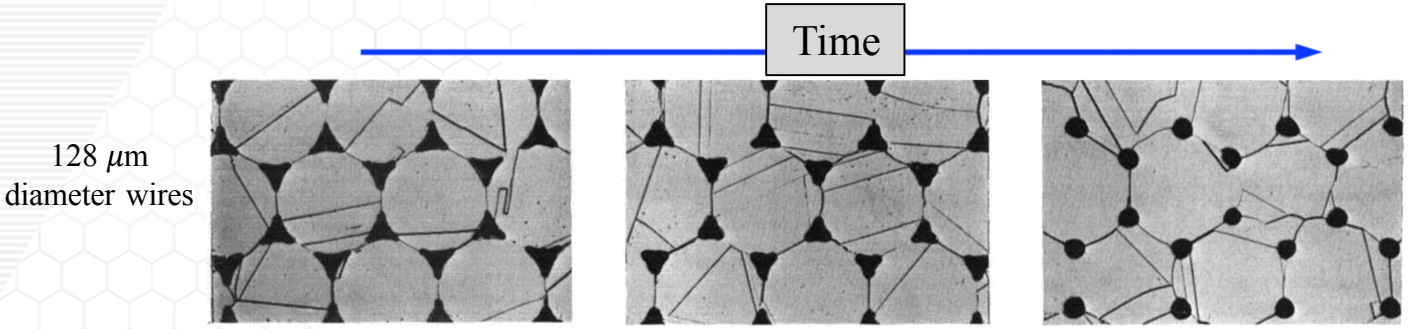
Broad materials compatibility

**Polymers** **Ceramics** **Metals**

# SINTERING: BASIC CONCEPTS

A heat treatment that leads to the consolidation of a powder compact by reduction of its surface area



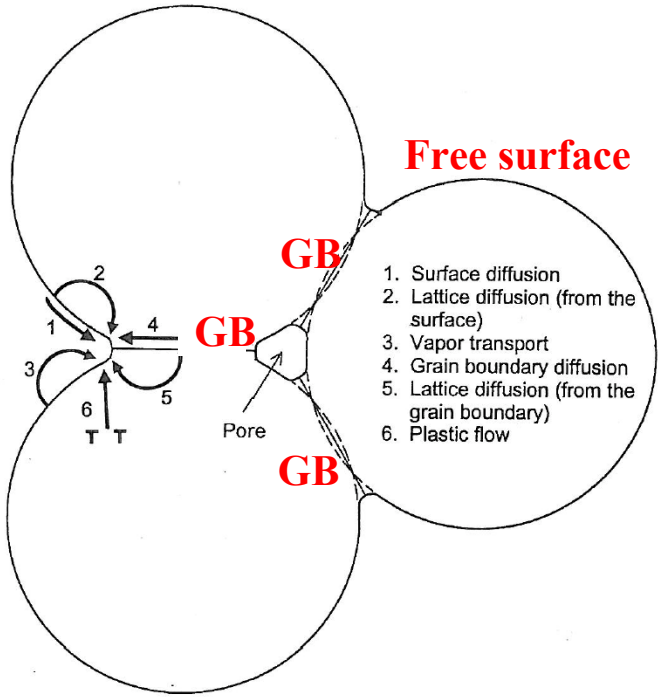




Alexander and Balluffi, Acta Metall. 5 (1957)

# SINTERING: BASIC CONCEPTS

- Solid-state process [~ 0.5 – 0.7 $T_m$]
- Two competing processes
  - **Densification**: reduction in porosity (shrinkage of body)
  - **Coarsening**: free surface evolution and grain growth processes

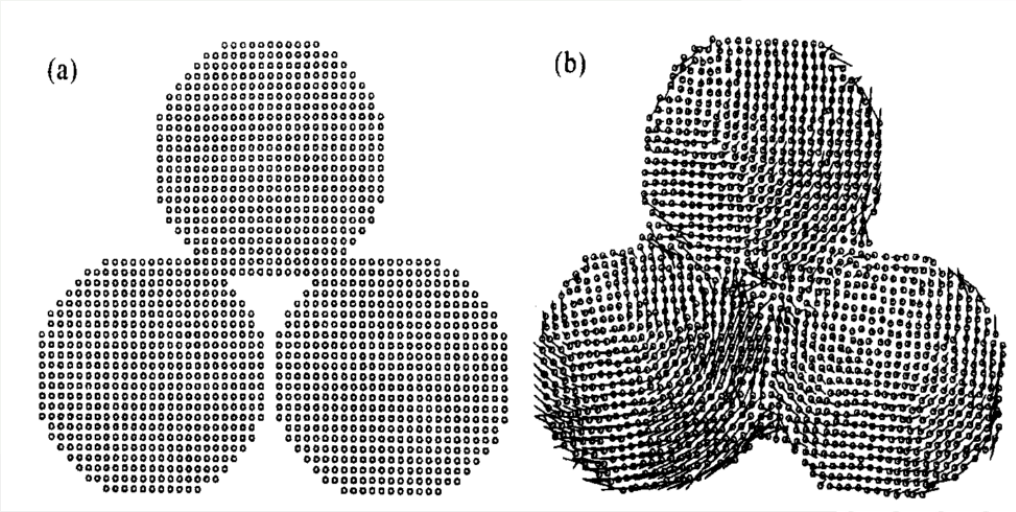
**Diffusional transport of matter**



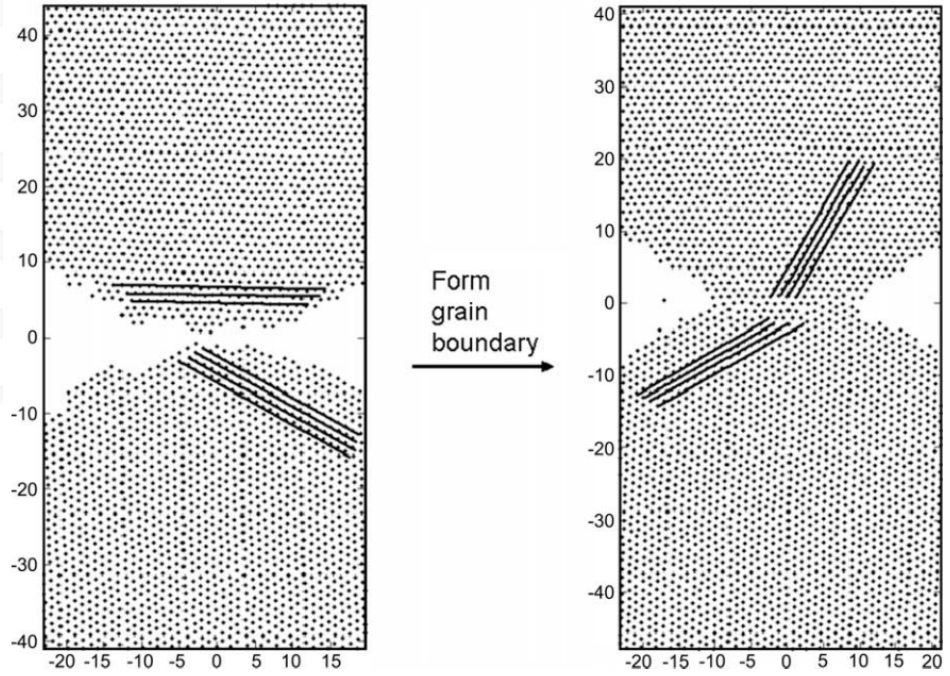

Rahaman, ceramic processing and sintering (2003)

# SINTERING: CURRENT RESEARCH

- Explored Pore Shrinkage to Measure Sintering
- Observed Grain Boundary Formation
- Observed Particle Reorientation



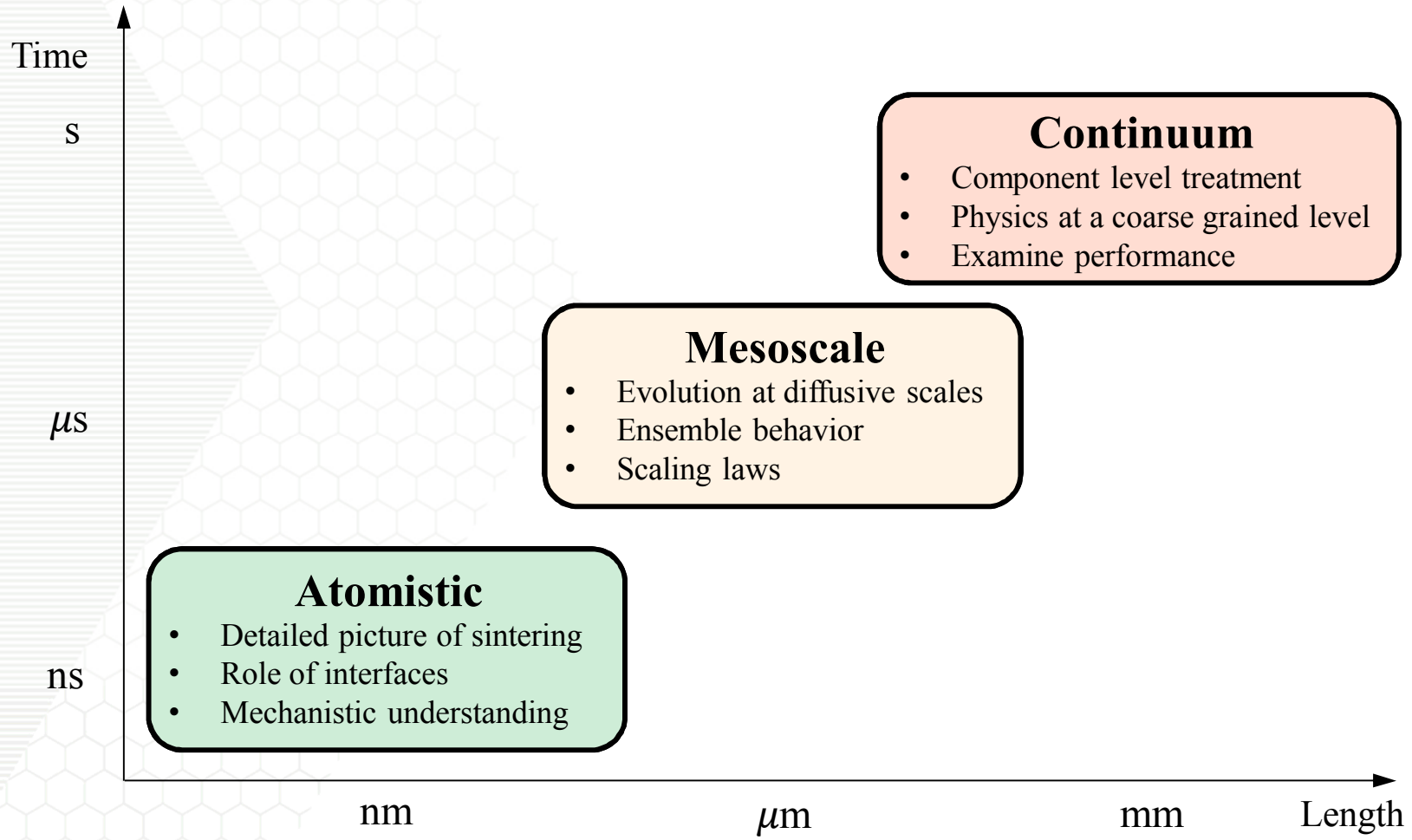

Zeng, P., Zajac, S., Clapp, P. C., & Rifkin, J. A. (1998). Nanoparticle sintering simulations. *Materials Science and Engineering A*, *252*(2)




Ding, L., Davidchack, R. L., & Pan, J. (2009). A molecular dynamics study of sintering between nanoparticles. Computational Materials Science, 45(2)

# MODELING CAPABILITIES AND APPROACH

- Sintering vs. Grain Boundary
  - Crystallographic reorientation
  - Grain Boundary formation and re-structuring
  - Pore shrinkage
  - Lattice distortion

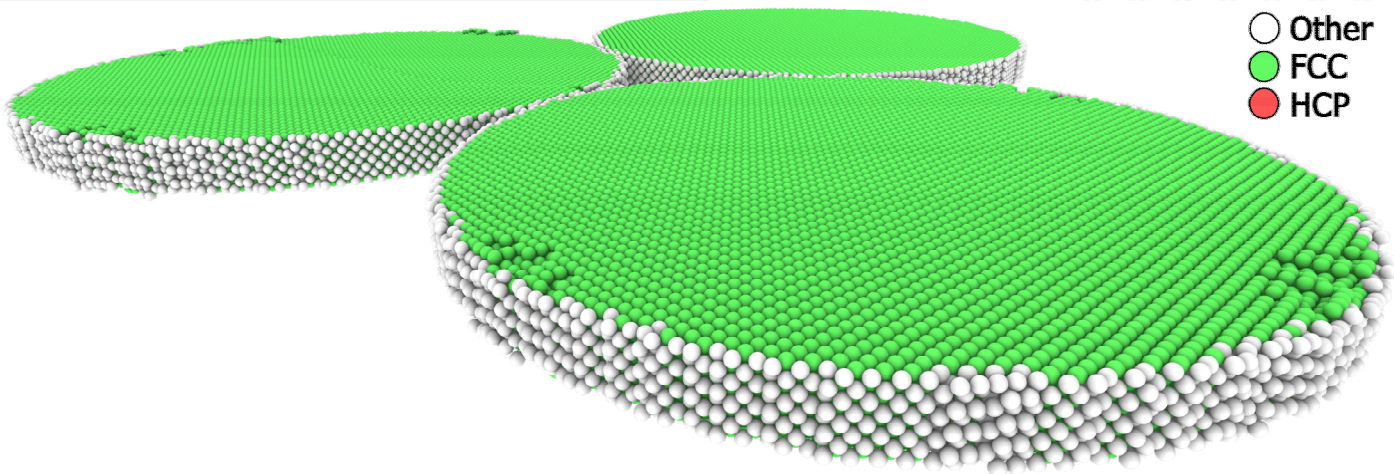


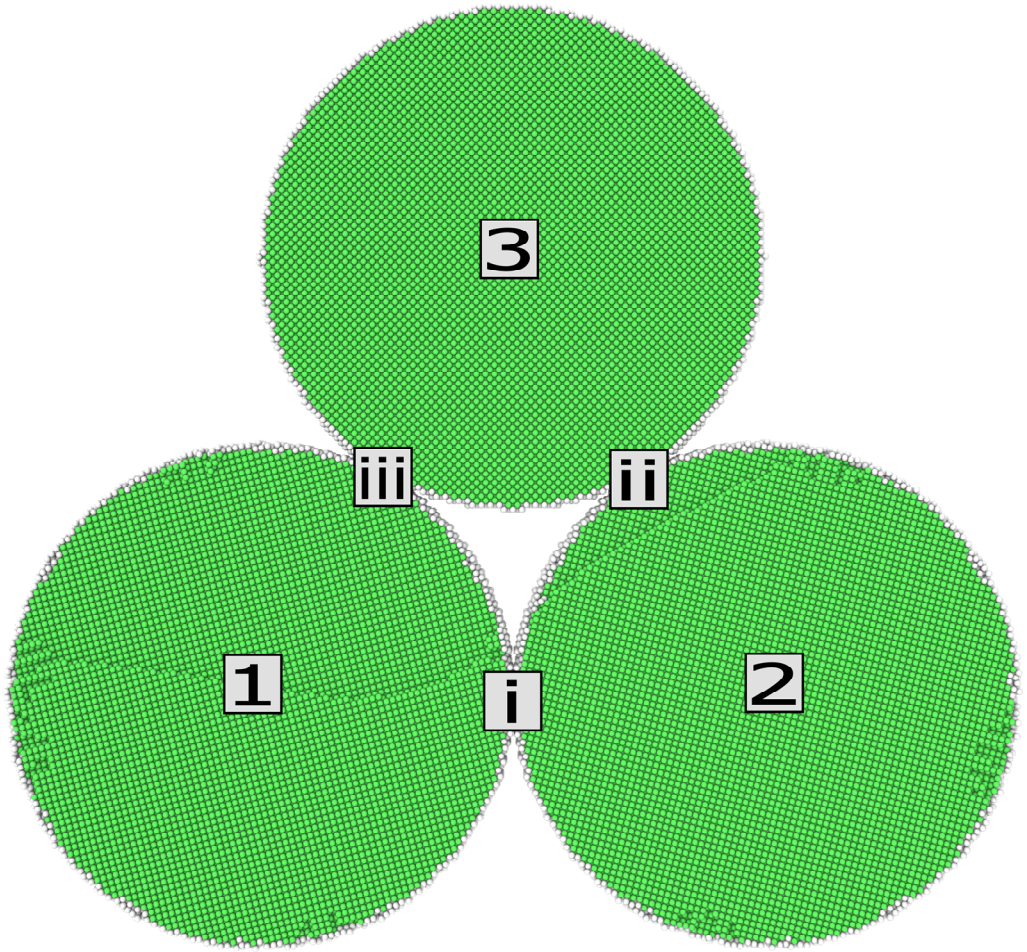
# EXPERIMENT SETUP

- Material: Nickel
- 2 and 3 Particle configurations
- Particle rotations along the z axis

**Molecular Dynamic Simulation**

- Box Relaxation
- Equilibration: NVT at 300K (0.5 ns)
- Ramp to Sintering Temperature: NVT (0.5 ns)
- Sinter: NVT at 1000K (40 ns)

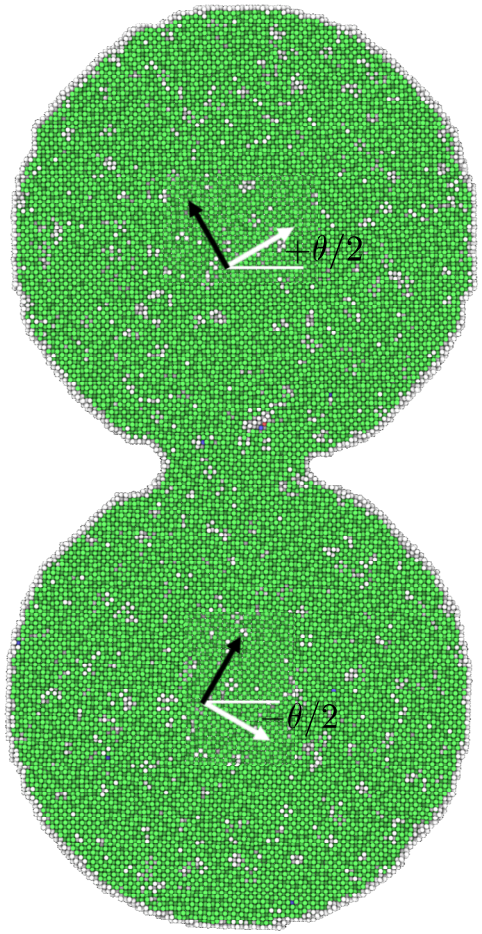


# 2-PARTICLE GEOMETRY

- Misorientation vs. Grain Boundary Formation
  - Lattice Orientation of x <1 0 0>, y <0 1 0>, z <0 0 1>
  - Vary 2r and Misorientation Angle systematically
  - With sizes ranging from X to Y

| | Misorientation Angle | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 2r | 5˚ | 10˚ | 15˚ | 20˚ | 25˚ | 30˚ | 35˚ | 40˚ | 45˚ |
| 5 nm | | | | | | | | | |
| 10 nm | | | | | | | | | |
| 20 nm | | | | | | | | | |
| 30 nm | | | | | | | | | |
| 40 nm | | | | | | | | | |

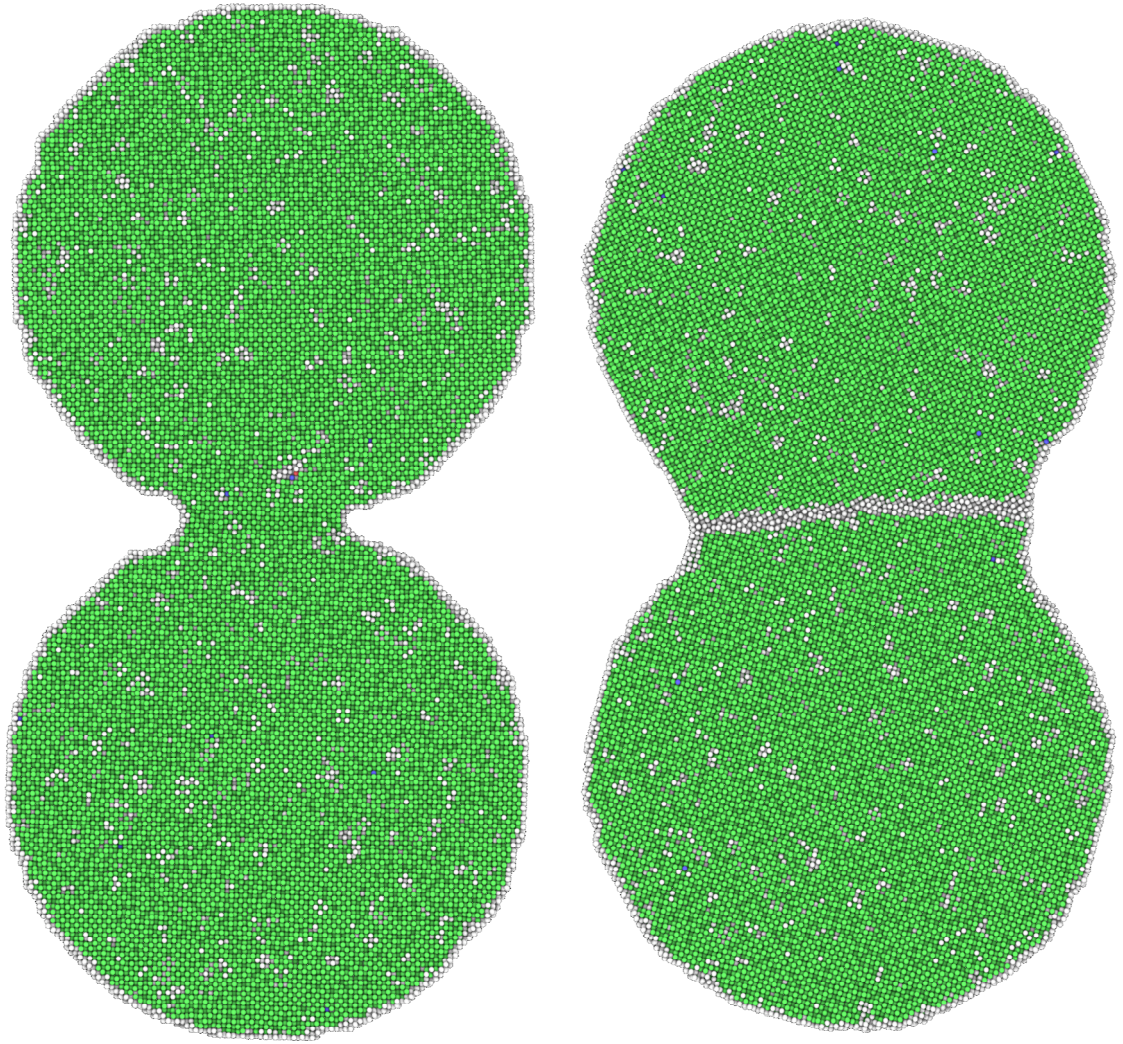


# 2-PARTICLE GEOMETRY

- Observations
  - Particle rotation along z-axis
  - GB formation increased neck size
  - GB formation increases
    - Misorientation Angle increases
    - Particle Diameter increases

| 2r | Misorientation Angle 5° | 10° | 15° | 20° | 25° | 30° | 35° | 40° | 45° |
|---|---|---|---|---|---|---|---|---|---|
| 5 nm | | | | | | | | | |
| 10 nm | | | | | | | | | |
| 20 nm | | | | | | | | | |
| 30 nm | | | | | | | | | |
| 40 nm | | | | | | | | | |

**Final Sinter**



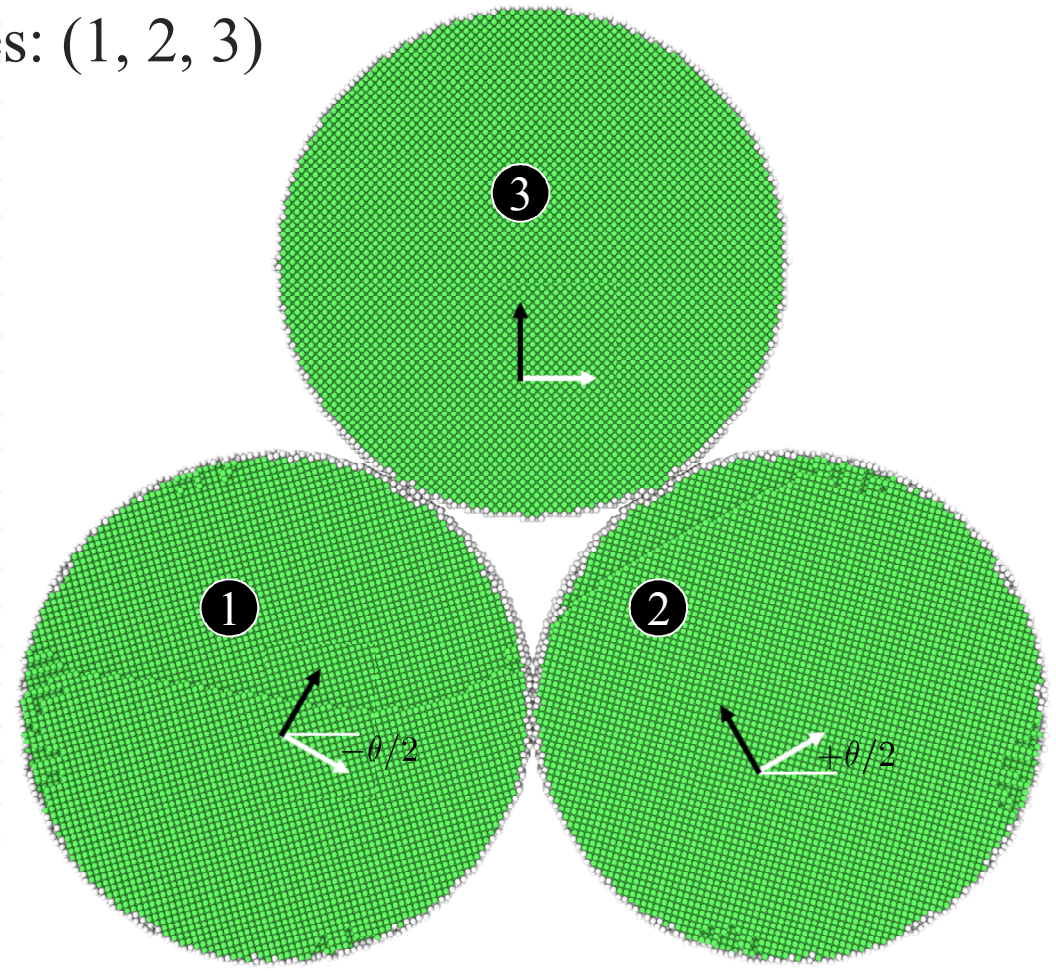
2r = 20 nm
$\theta$ = 20˚

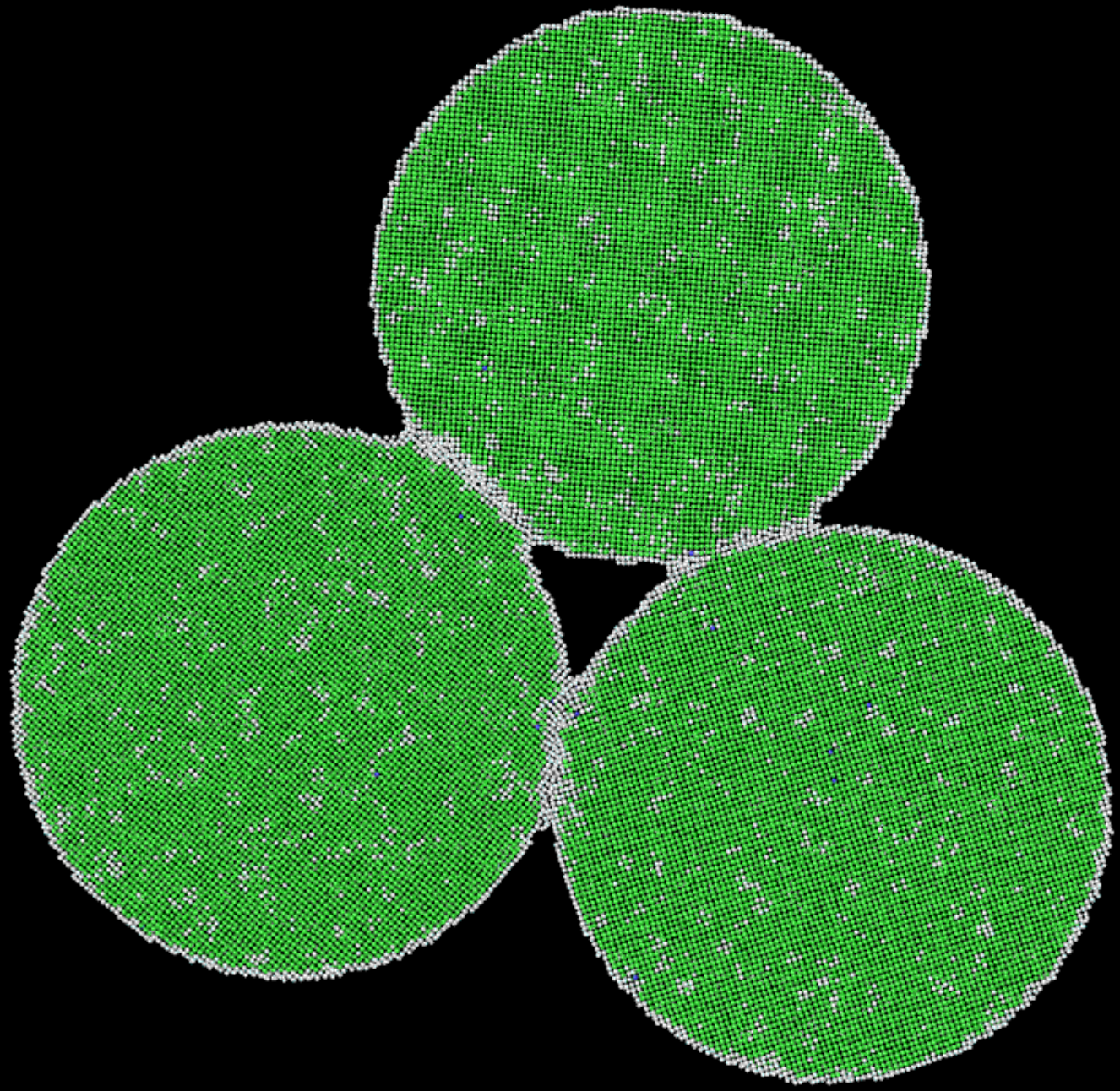
2r = 20 nm
$\theta$ = 40˚

# 3-PARTICLE GEOMETRY

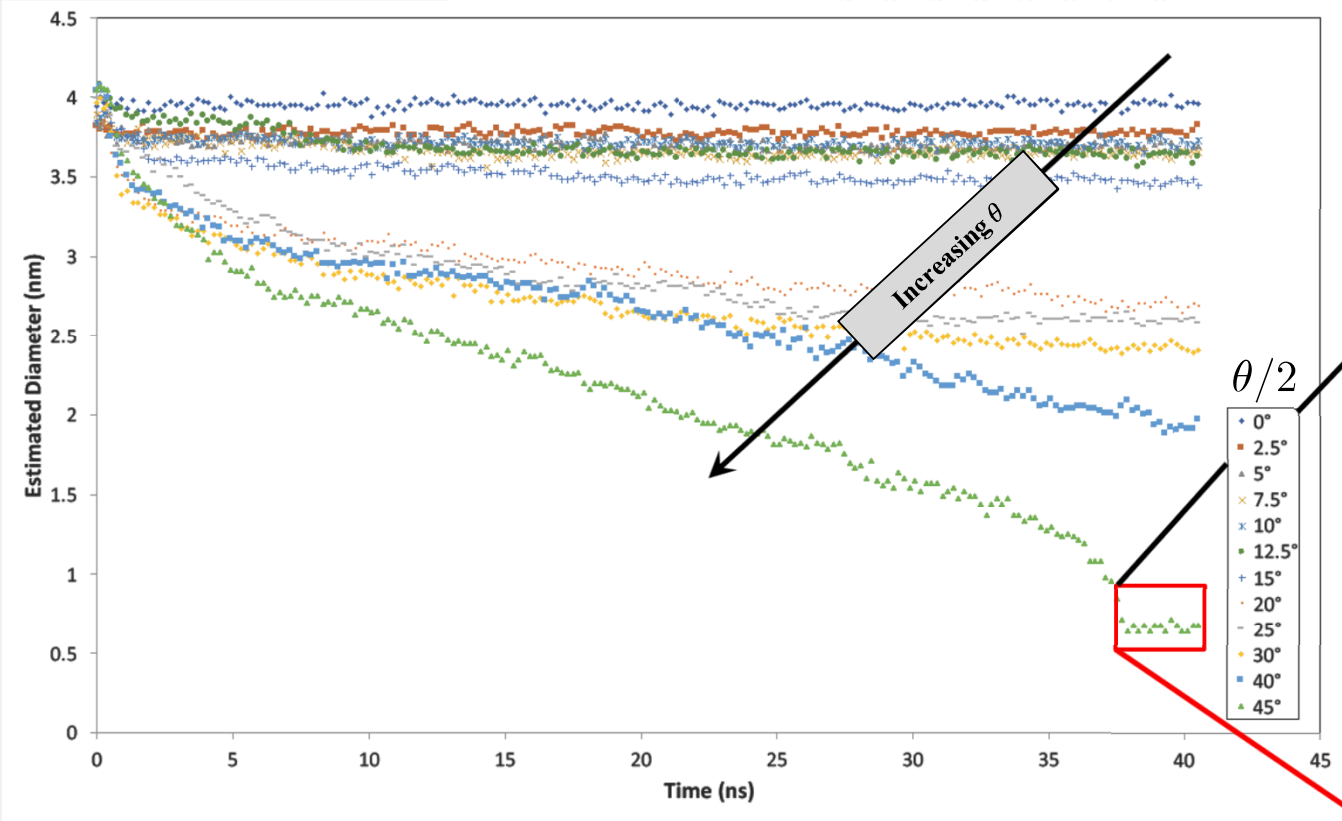
- Shrinkage vs. Grain Boundary
  - Z axis rotations are: $(-\theta/2, +\theta/2, 0)$ for particles: $(1, 2, 3)$
  - Lattice Orientations
    - x <1 0 0>, y <0 1 0>, z <0 0 1> Max $\theta/2$: 45˚
    - x <1 -1 4>, y <2 -2 -1>, z <1 1 0> Max $\theta/2$: 90˚
    - x <2 -1 -1>, y <0 1 -1>, z <1 1 1> Max $\theta/2$: 60˚
  - One $\theta$ GB and Two $\theta/2$ GB
  - Vary Lattice Orientation and Particle Misorientation

$$\text{Shrinkage} = \frac{A_{pore}(0) - A_{pore}(t)}{A_{pore}(0)}$$

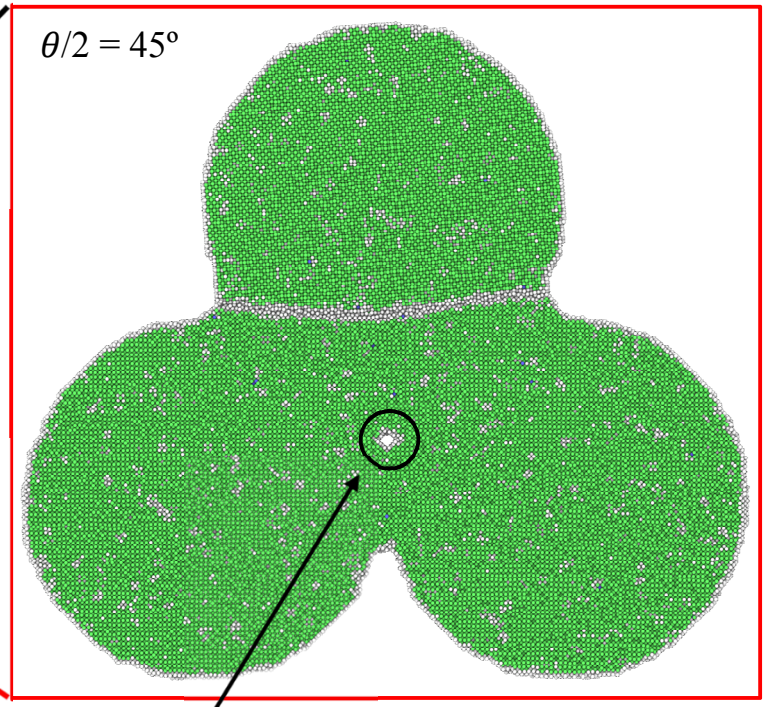




# 3-PARTICLE GEOMETRY: PORE SIZE




**GB Break-away event**

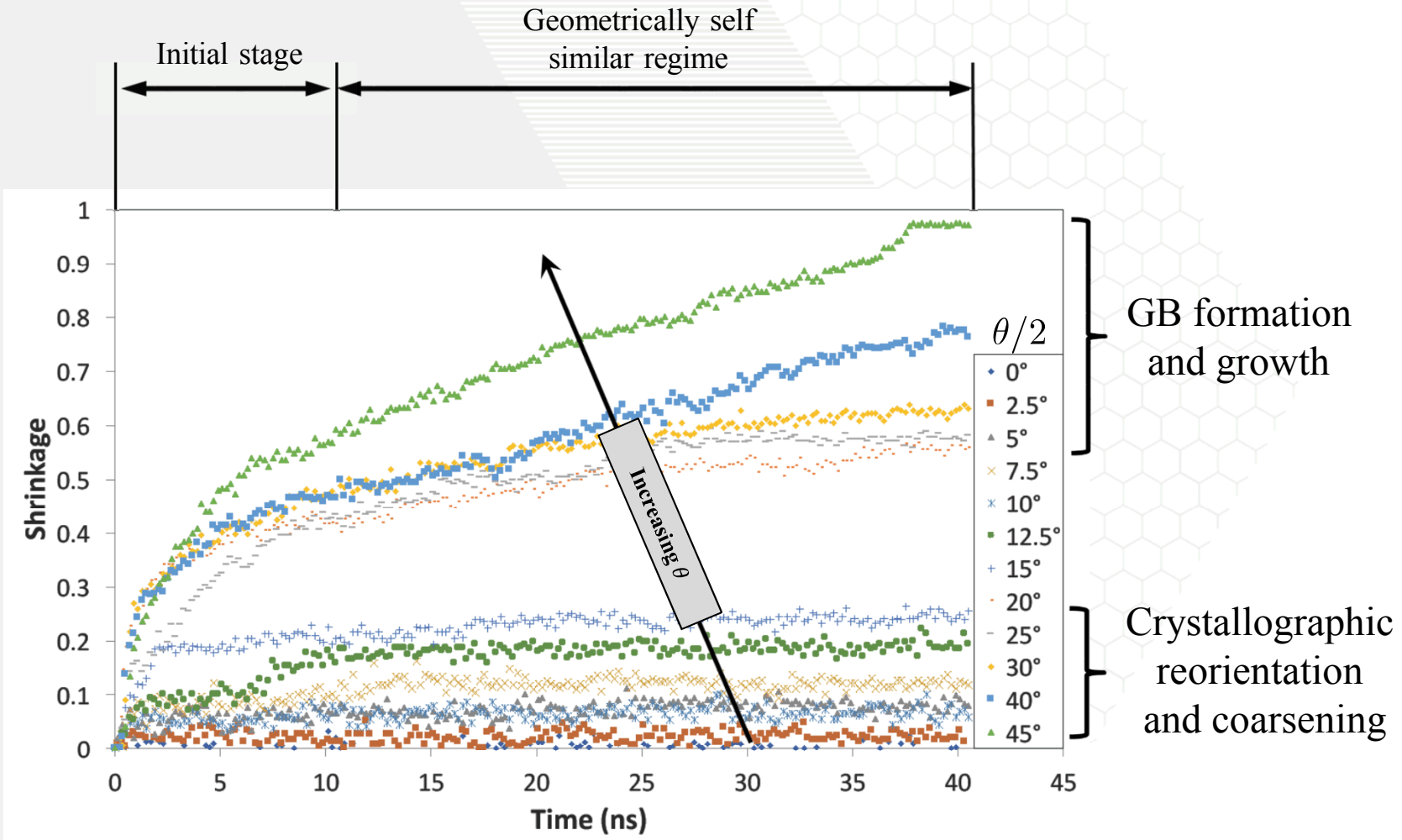



Pore left behind

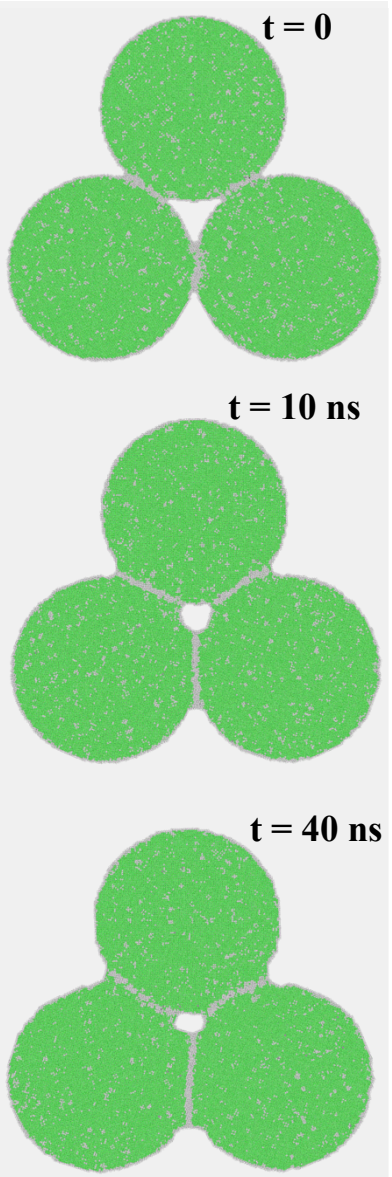
**Observations:**

- Stagnant behavior at low $\theta$
- Rapid pore shrinkage at large $\theta$
- Self similar behavior after an initial transient

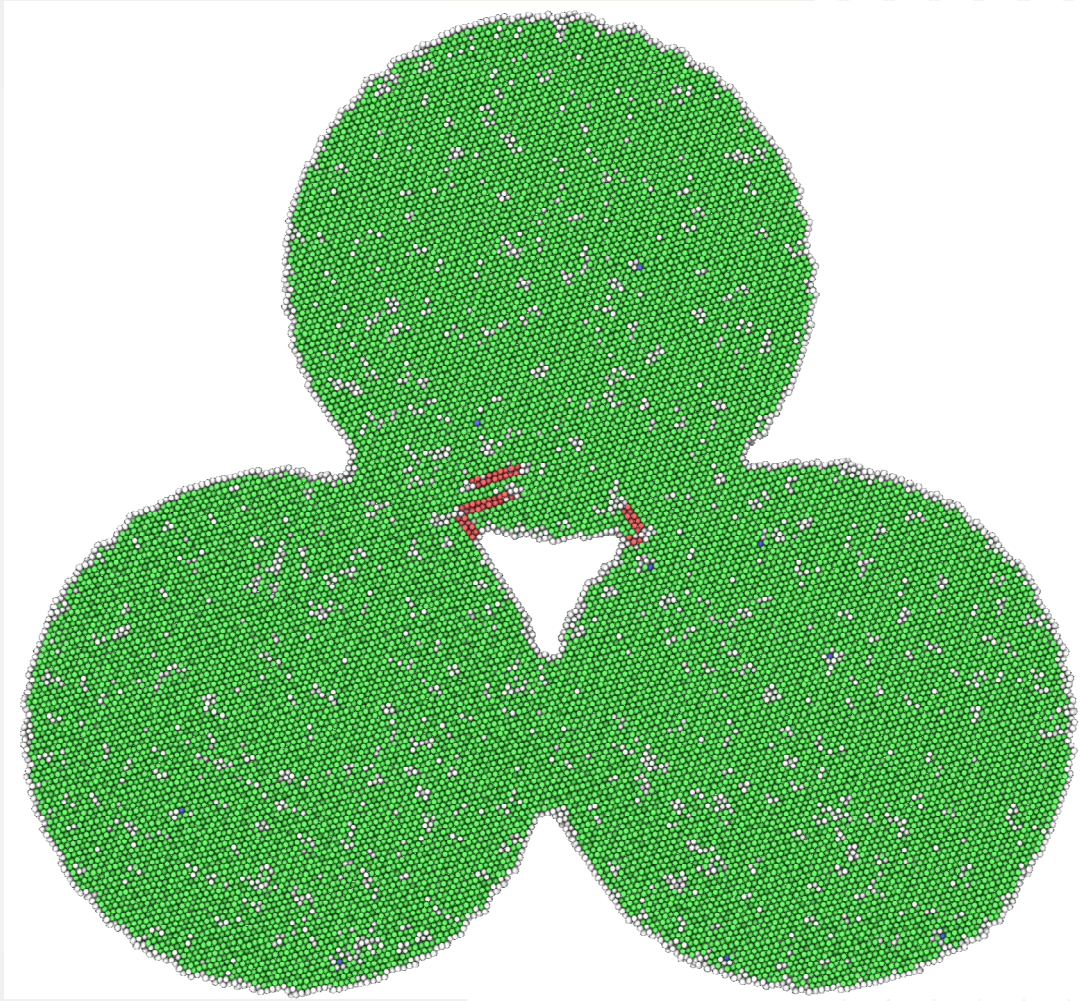
# 3-PARTICLE GEOMETRY: SHRINKAGE



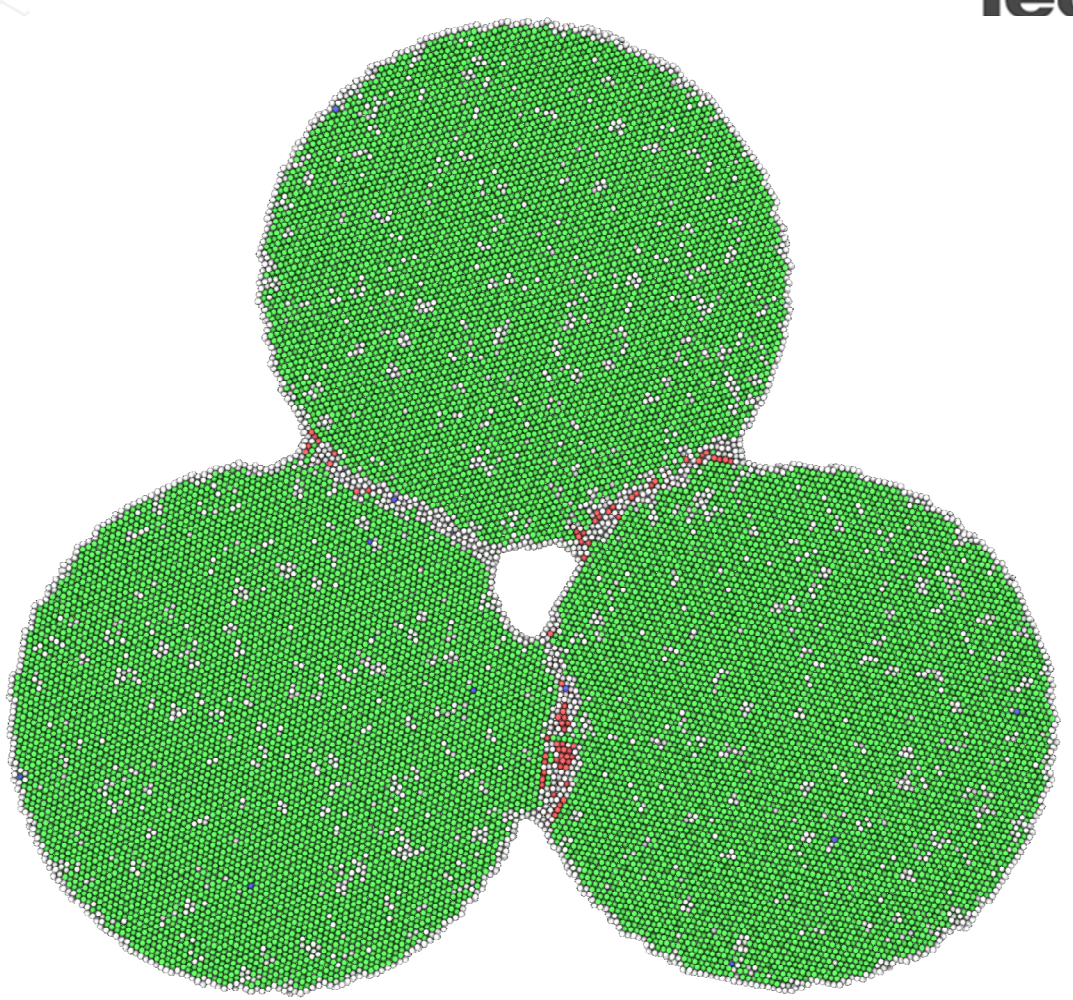

$\theta/2 = 30°$



# EXPANDING LATTICE ORIENTATIONS – Z <1 1 0>



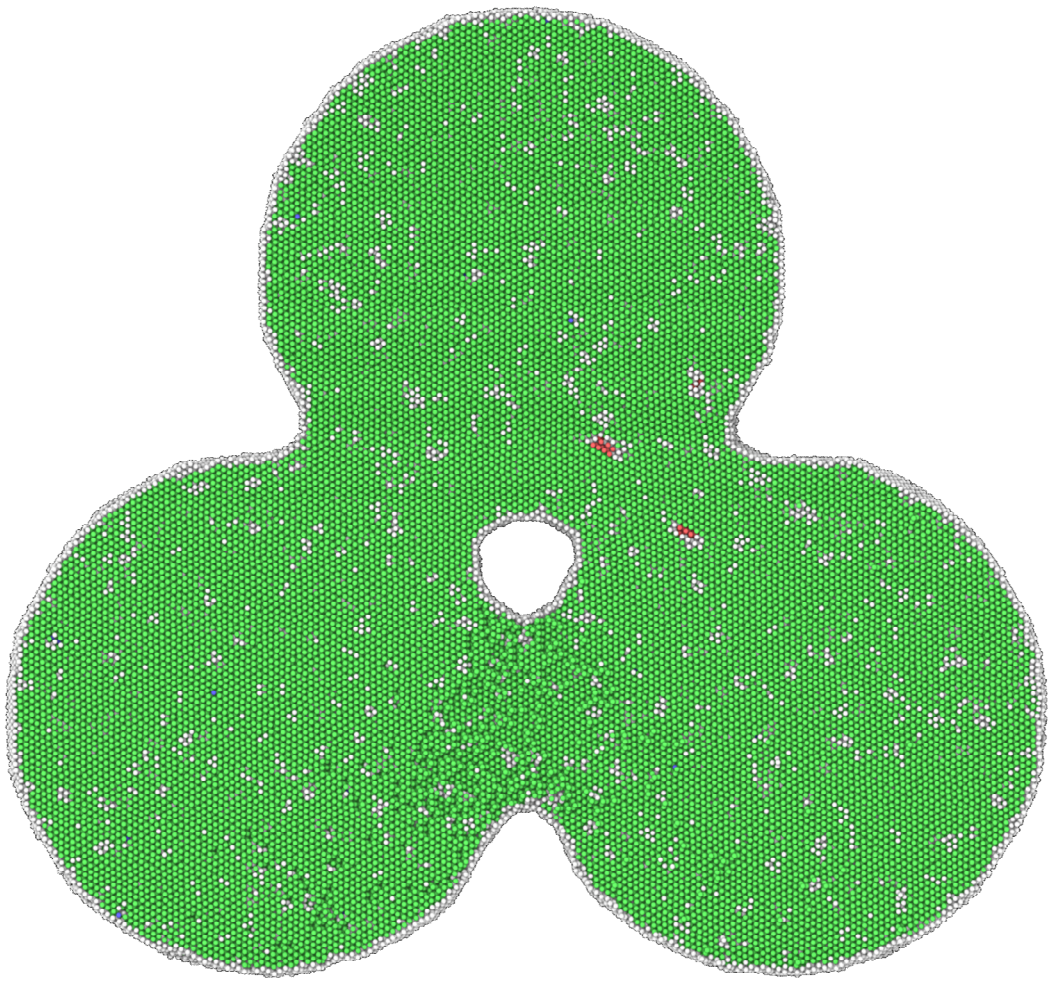
$\theta/2 = 0^{\circ}$



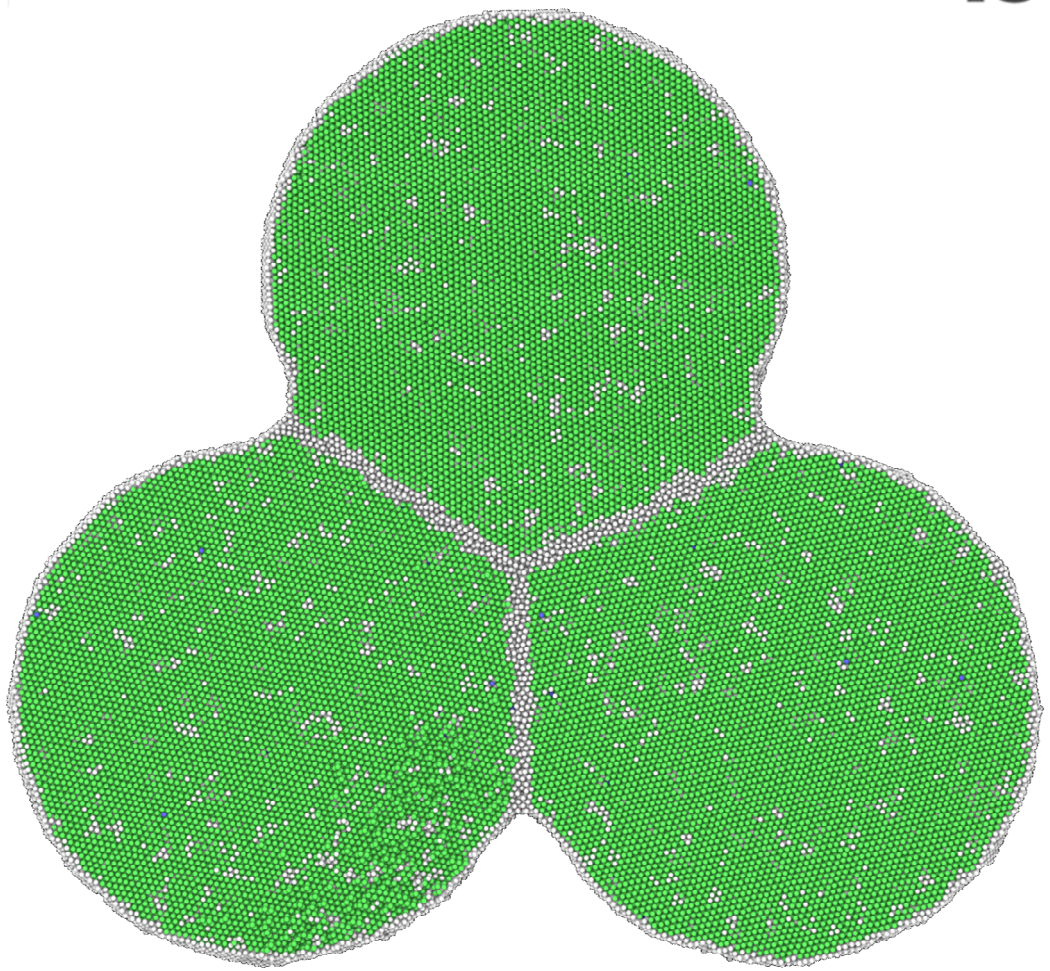
$\theta/2 = 40^{\circ}$

**Final Sinter**

# EXPANDING LATTICE ORIENTATIONS – Z <1 1 1>



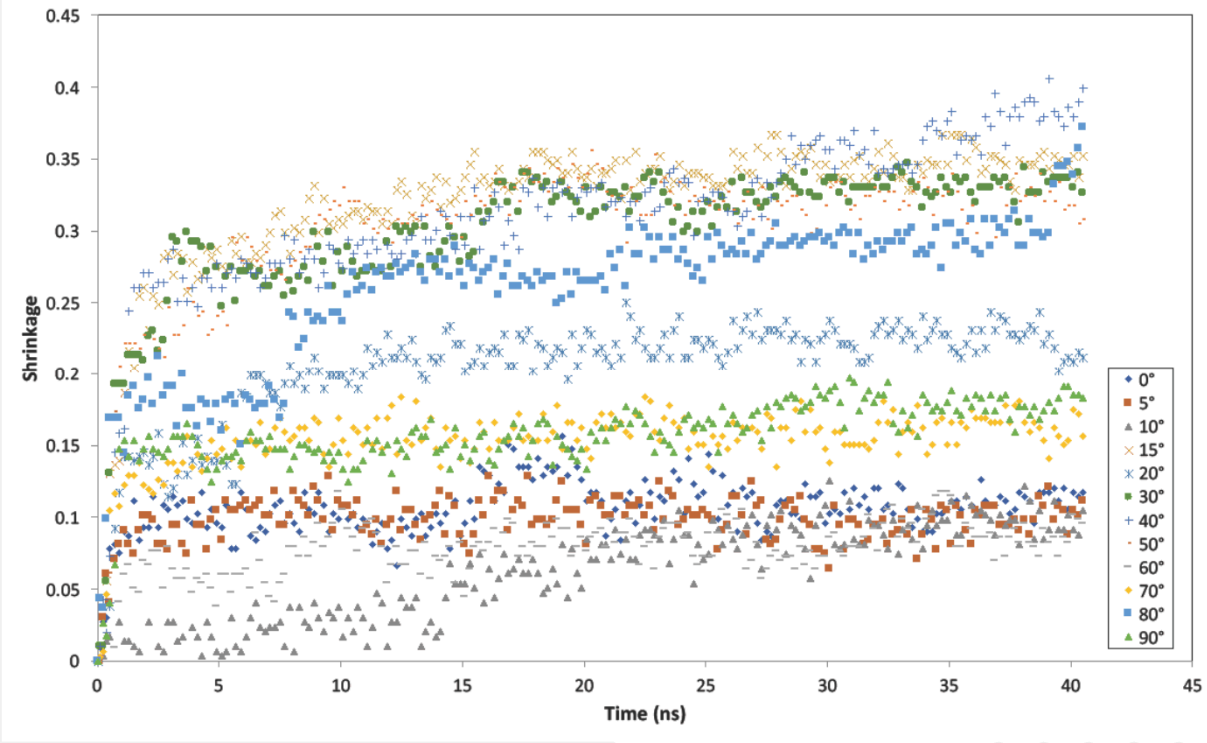
$\theta/2 = 0^{\circ}$



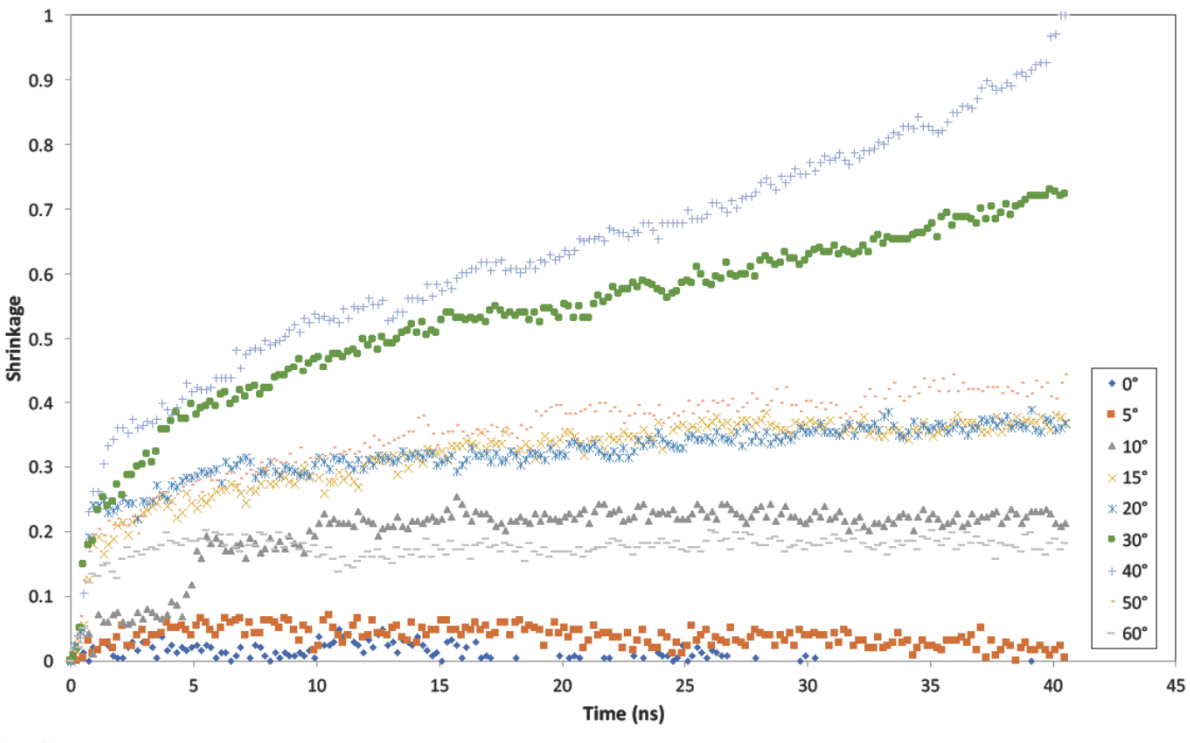
$\theta/2 = 40^{\circ}$

**Final Sinter**

# EXPANDING LATTICE ORIENTATION - SHRINKAGE



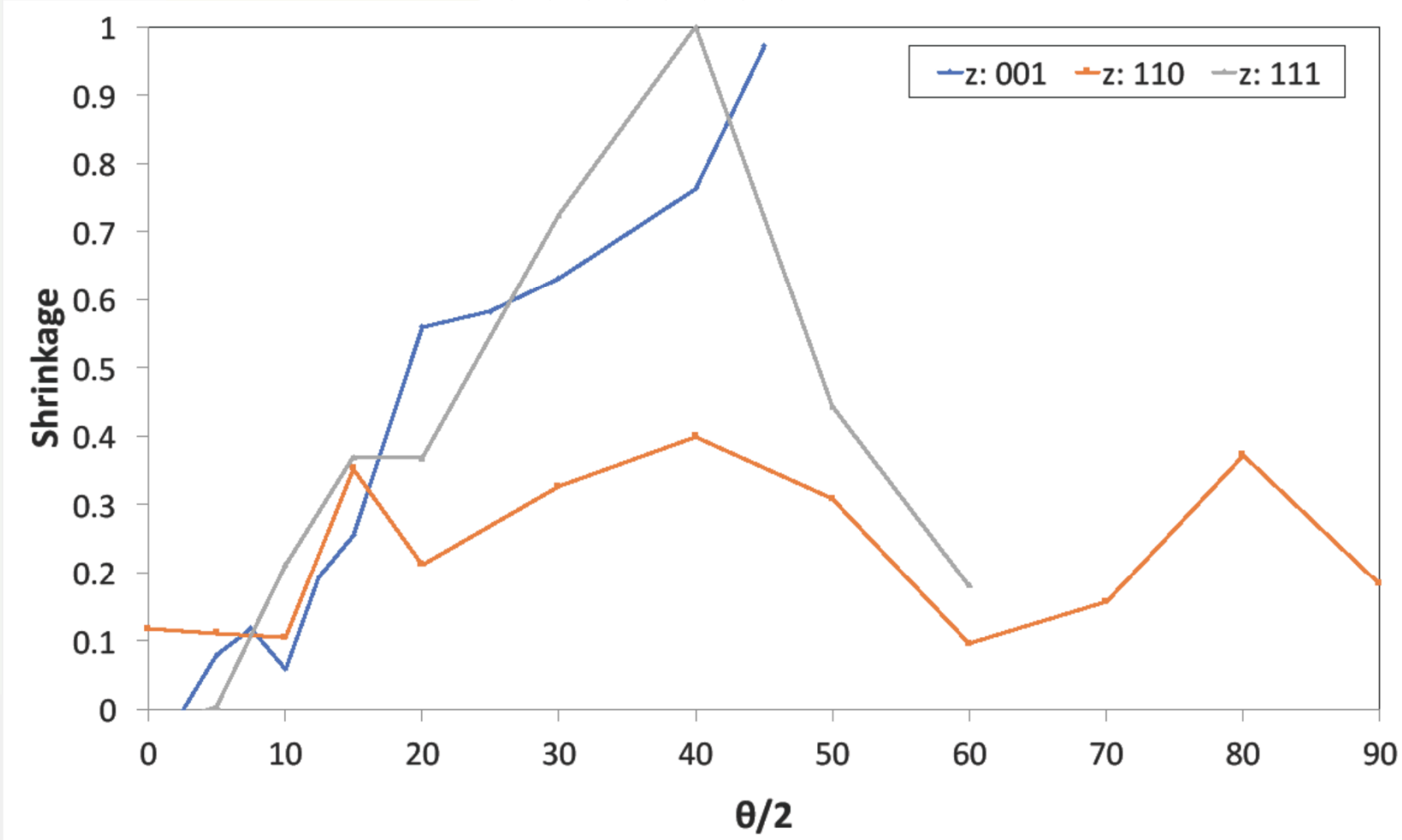

Z <1 1 0>




Z <1 1 1>

# ESTABLISHING RELATIONSHIP

- GB Type vs. Pore Shrinkage



# OBSERVATIONS AND CONCLUSION

- Observed similar physical characteristics

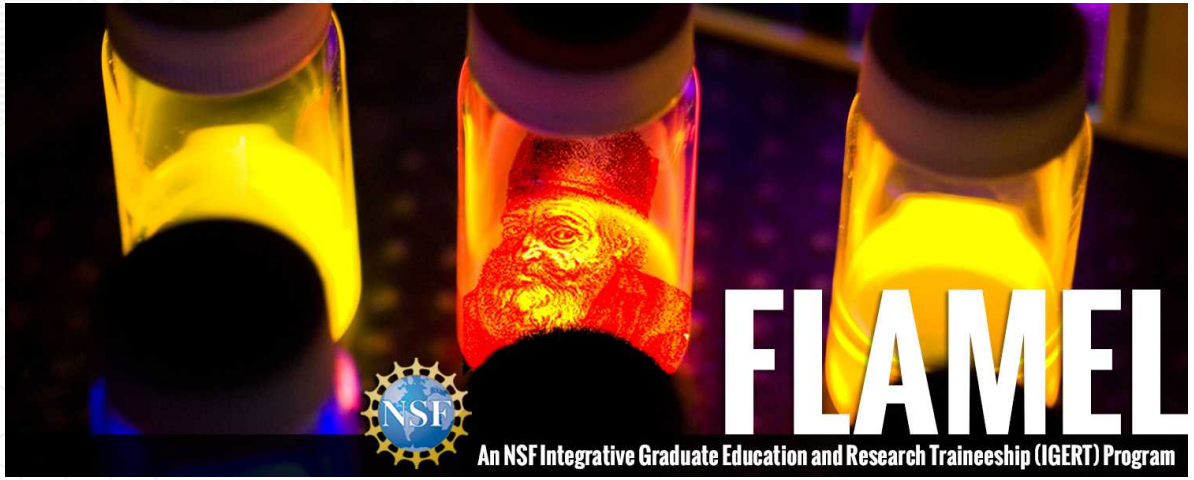
- Particle Reorientation
  - Both the two and three particle simulations
  - Occurred during Equilibration, Ramp, and Sintering steps
  - This affected grain boundary formation and growth

- Establish relationship between grain boundary versus pore shrinkage

# ACKNOWLEDGMENTS

Georgia Tech

Sandia National Laboratories



# BACKUP SLIDES

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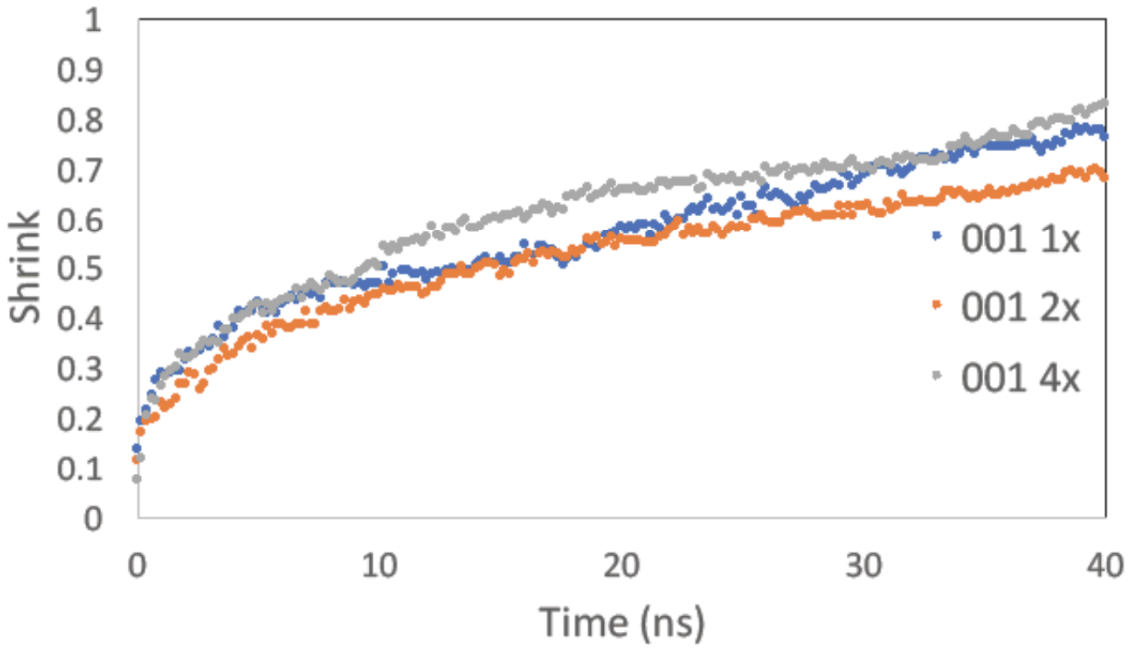
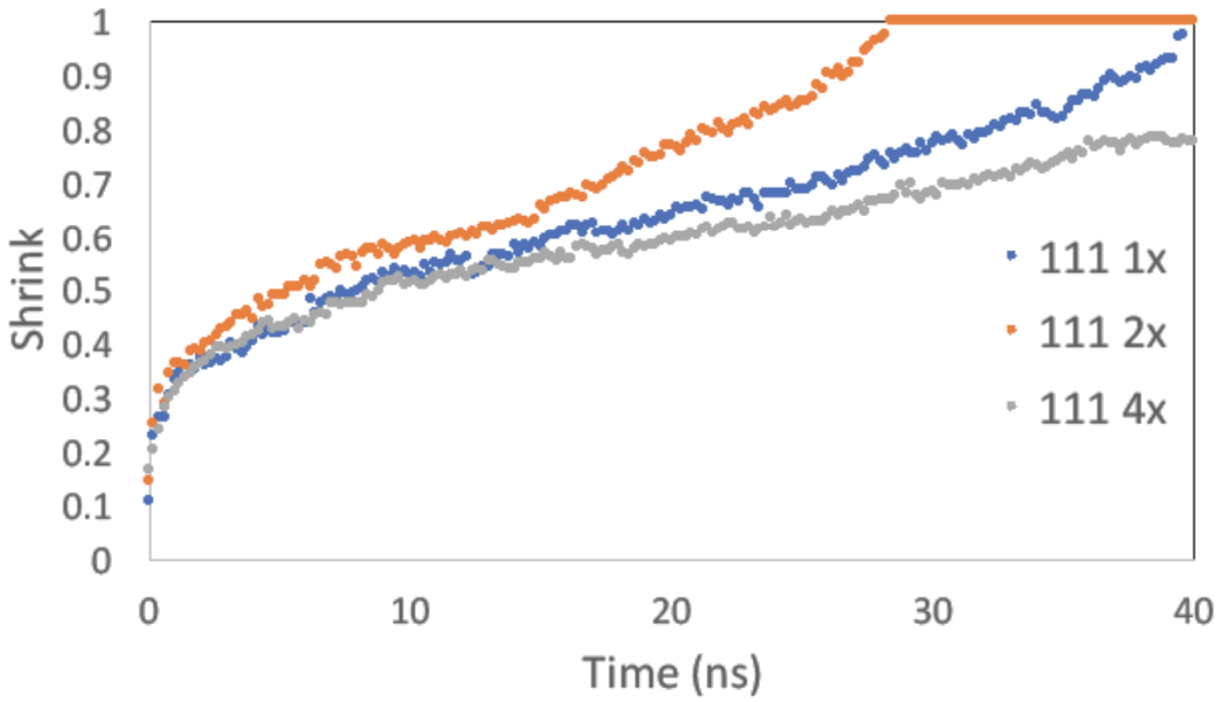
# Z THICKNESS VARIATION



# LOG-LOG RELATIONSHIP FOR Z <1 1 1>