

Tracking Microstructural Evolution in Simulations of Recrystallization

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E. A. Holm

¹Sandia National Laboratory

²University of Florida

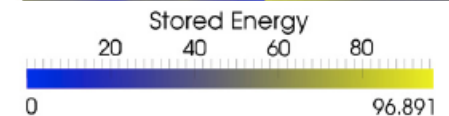
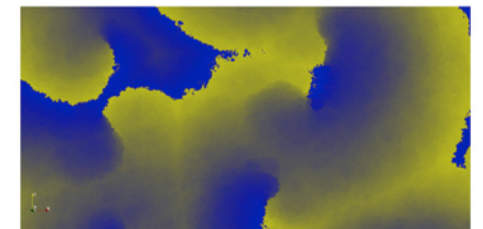
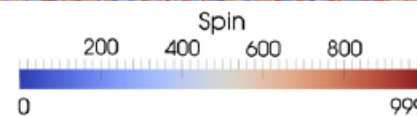
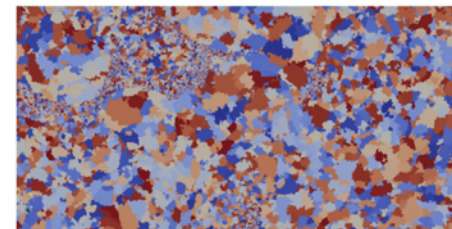
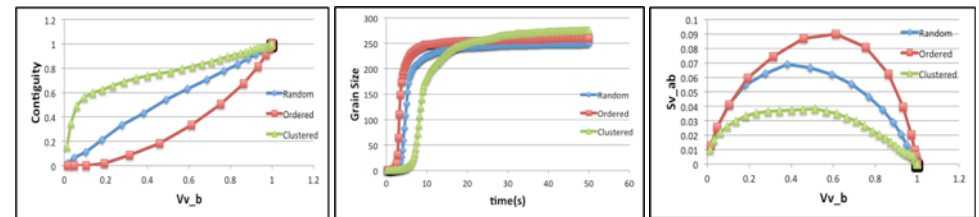
³Carnegie Mellon University



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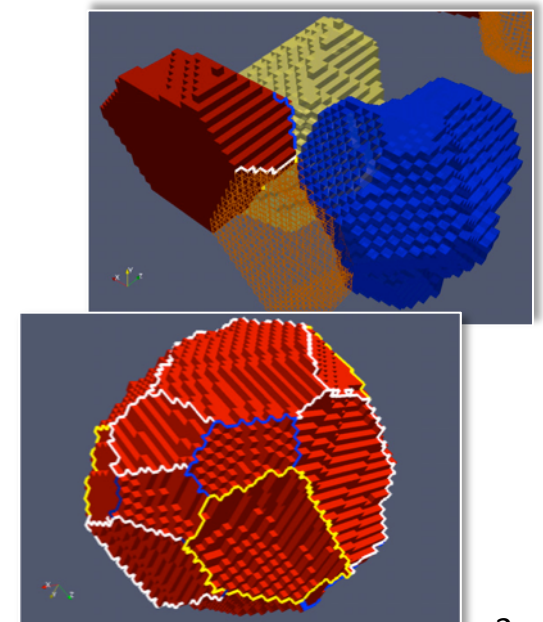
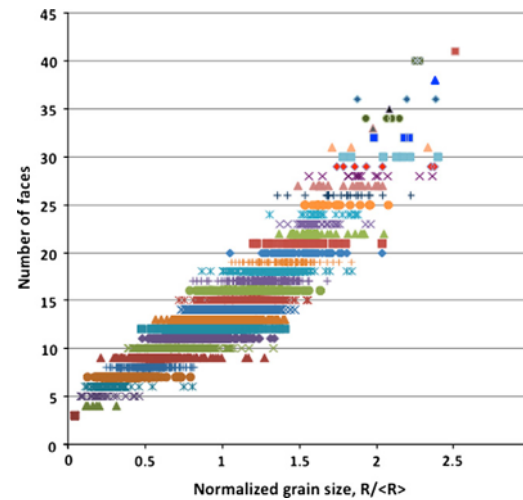
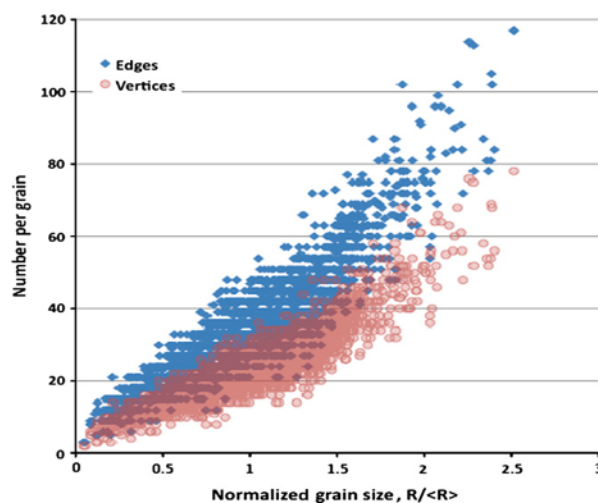


Outline

- Background
- Simulation Framework
- Algorithm Components
 - Kinetic Monte Carlo for Grain Growth
 - Cellular Automata for Recrystallization
 - Nuclei Instantiation & Insertion
- Tracked Parameters
 - Grain Size & Volume Fraction
 - Interfacial Surface Area
 - KJMA Exponent
 - Contiguity
 - Ordering Influence on Grain Size Distributions
- Future Work
- Conclusions

Background I

- Topological changes during grain growth are thought to control microstructural evolution
- Here we apply a recently developed automated method❖ to characterize topology in digital microstructures, to simulations of 2D static recrystallization

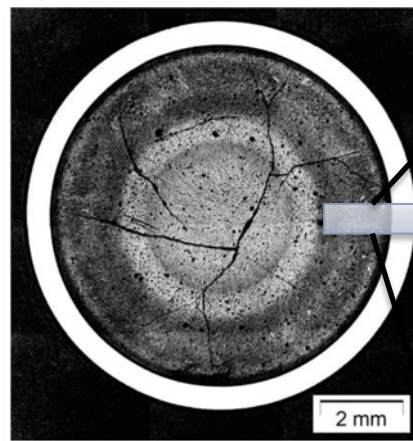


- ❖ Z. Sun, V. Tikare, B. R. Patterson and A. P. Sprague: *Comp. Mat. Sci.*, 2012, vol. 55 pp. 329-36.

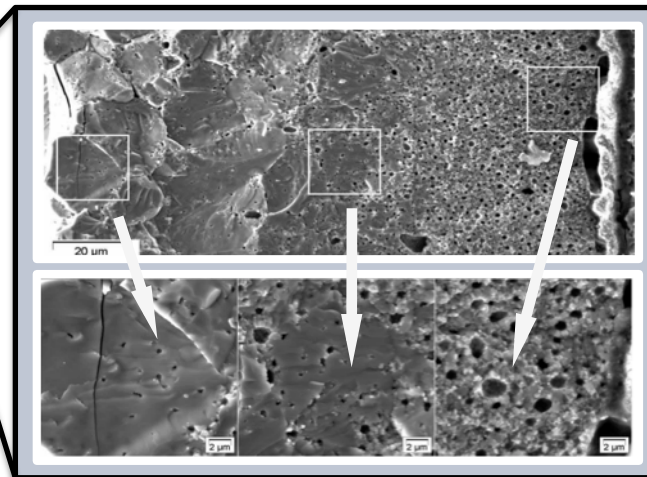
Background II

- We are interested in recrystallization for 2 primary reasons
 - Common occurrence in engineered metals undergoing large-scale deformation (e.g. rolling)
 - Proposed as the evolutionary process responsible for the 'rim effect' in nuclear fuels

Nuclear Fuel Pellet
www.nrc.gov



Irradiated Fuel Cross-Section
Noiro, et. al NE&T, vol. 41 2009



RESULT

Tremendous Variation In Microstructure

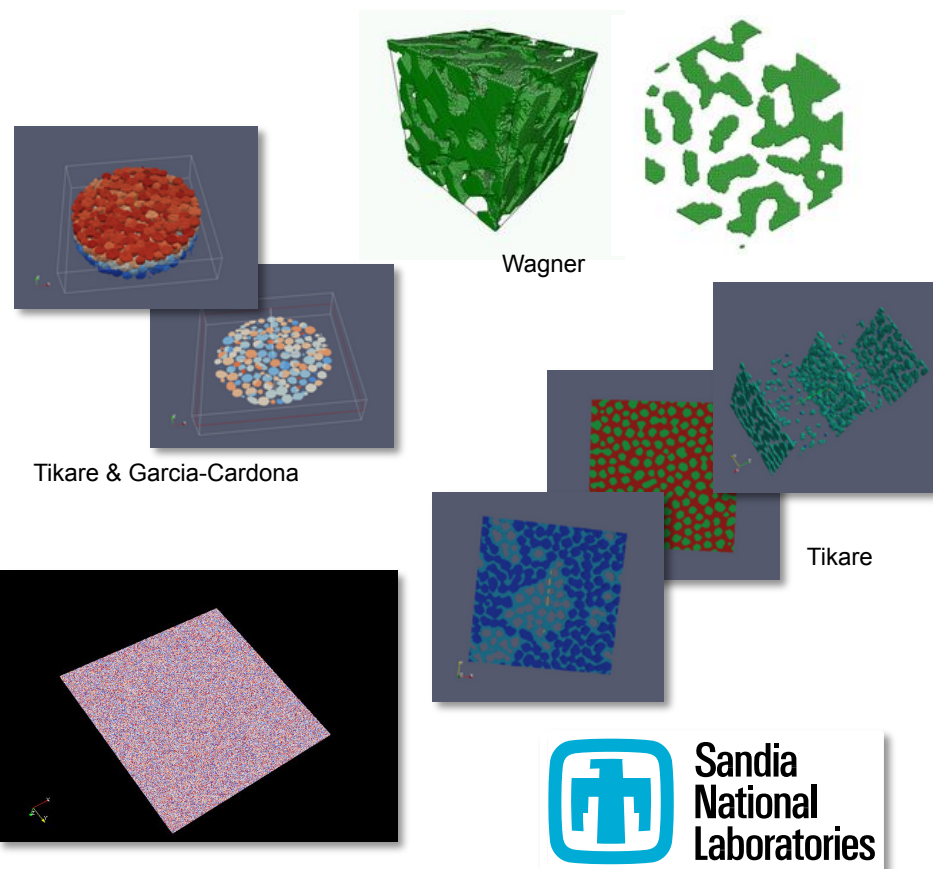
1. Grain size
2. Porosity
3. Percolation
3. Composition
4. Hardness

Simulation Framework

SPPARKS

Kinetic Monte Carlo via Stochastic Parallel PARticle Kinetic Simulator

- Development a new user application for SNL's SPPARKS open-source environment
- Treat grain growth + dynamic recrystallization events simultaneously
- Incorporate probabilistic cellular-automaton approach to more accurately capture realistic kinetics (KJMA rates)
- Toward prediction of microstructural evolution in irradiated materials beyond currently established NRC regulations



Algorithm Components

KINETIC MONTE CARLO

+

CELLULAR AUTOMATA

Stochastic, probability driven evolution

Deterministic, rule-based evolution

C.C. Battaile, The Kinetic Monte Carlo Method: Foundation, Implementation, and Application, Computer Methods in Applied Mechanics and Engineering, 197 (2008) 3386-3398.

H. Barreto, F.M. Howland, Introductory Econometrics: Using Monte Carlo Simulation with Microsoft Excel, Cambridge University Press, New York, 2006.

H.T. MacGillivray, R.J. Dodd, Monte-Carlo Simulations of Galaxy Systems II: Static Properties for Galaxies in Rich Clusters, Astrophysics and Space Science, 83 (1982) 127-142.

H.T. MacGillivray, R.J. Dodd, B.V. McNally, J.F. Lightfoot, H.G. Corwin Jr, S.R. Heathcote, Monte-Carlo Simulations of Galaxy Systems I: The Local Supercluster, Astrophysics and Space Science, 81 (1982) 231-250.

D.K. Umberger, J.D. Farmer, I.I. Satija, A Universal Strange Attractor Underlying the Quasiperiodic Transition to Chaos, Physics Letters A, 114 (1986) 341-345.

P. Landau, K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, 2nd ed., Cambridge University Press, Cambridge, 2005.

A.D. Rollett, P. Manohar, The Monte Carlo Method, in: D. Raabe, F. Roters, F. Barlat, C. Long-Qing (Eds.) Continuum Scale Simulation of Engineering Materials, Wiley-VCH, Strauss GmbH, Morlenbach, 2004, pp. 77-114.

[37] K. Janssens, Cellular Automata, in: K.G.F. Janssens, D. Raabe, E. Kozeschnik, M.A. Miodownik, B. Nestler (Eds.) Computational Materials Engineering: An Introduction to Microstructure Evolution, Elsevier, Inc., Burlington, MA, 2007, pp. 109-150.

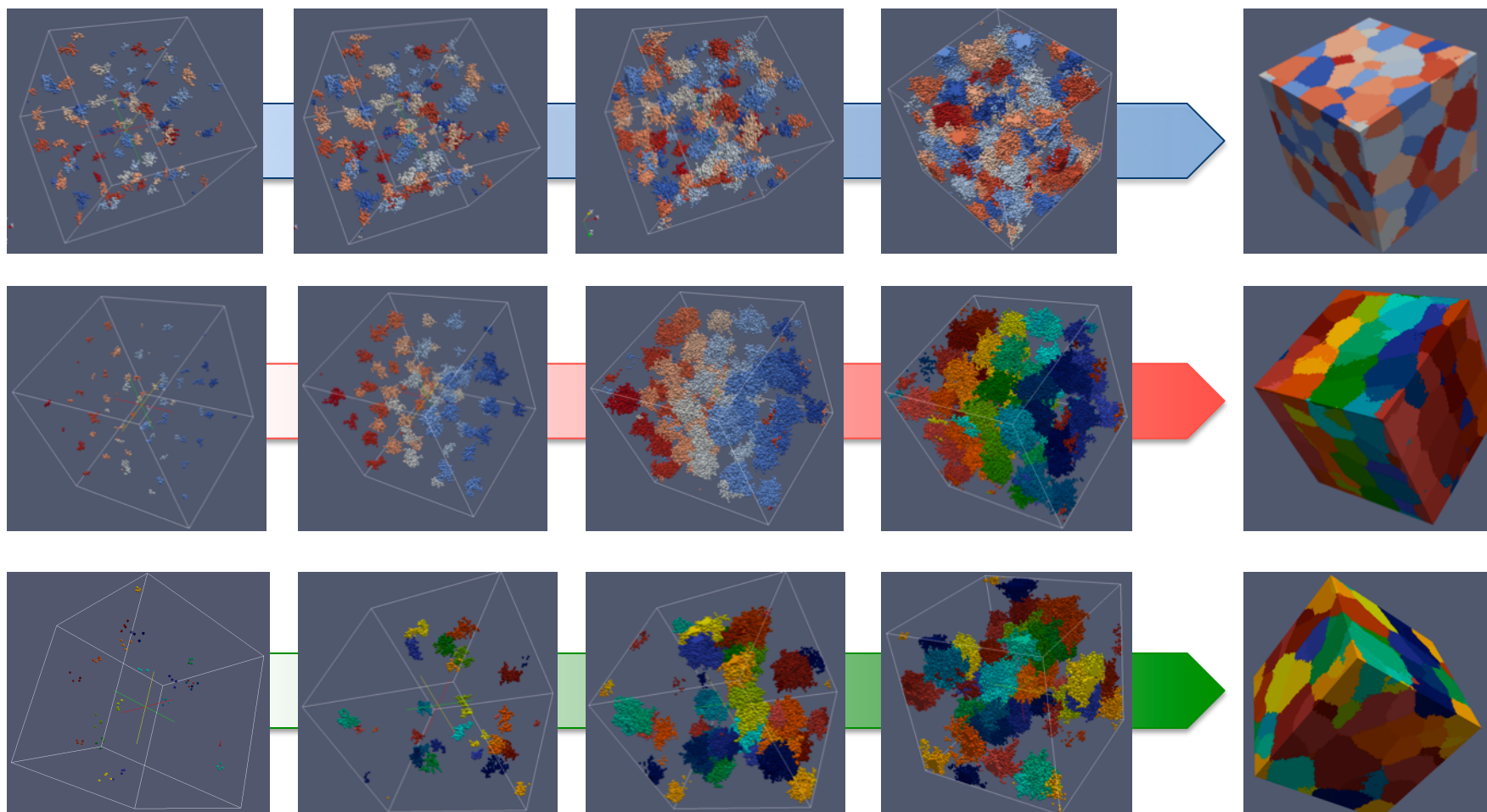
[38] D. Raabe, Cellular, Lattice Gas, and Boltzmann Automata, in: D. Raabe, F. Roters, F. Barlat, L.-Q. Chen (Eds.) Continuum Scale Simulation of Engineering Materials: Fundamentals-Microstructures-Process Applications, Wiley-VCH, Strauss GmbH, 2004, pp. 57-76.

[39] D. Raabe, Yield Surface Simulation for Partially Recrystallized Aluminum Polycrystals on the Basis of Spatially Discrete Data, Computational Materials Science, 19 (2000) 13-26.

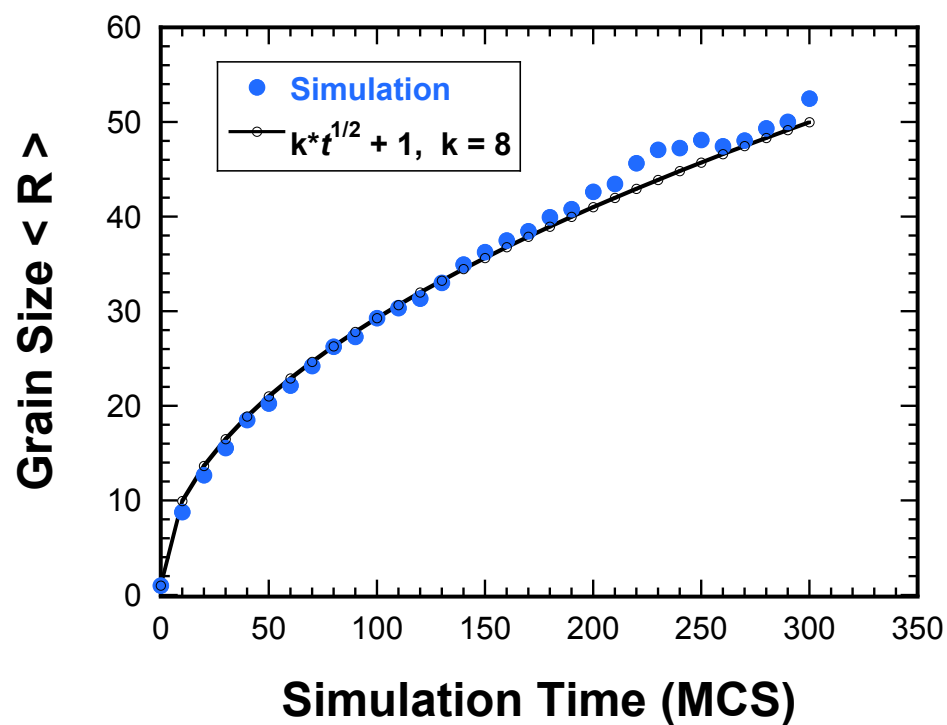
[40] D. Raabe, Mesoscale Simulation of Recrystallization Textures and Microstructures, Advanced Engineering Materials, 3 (2001) 745-752.

Nuclei Instantiation

Nuclei are “seeded” into the simulation domain in one of three ways;
1) random, 2) ordered, or 3) clustered

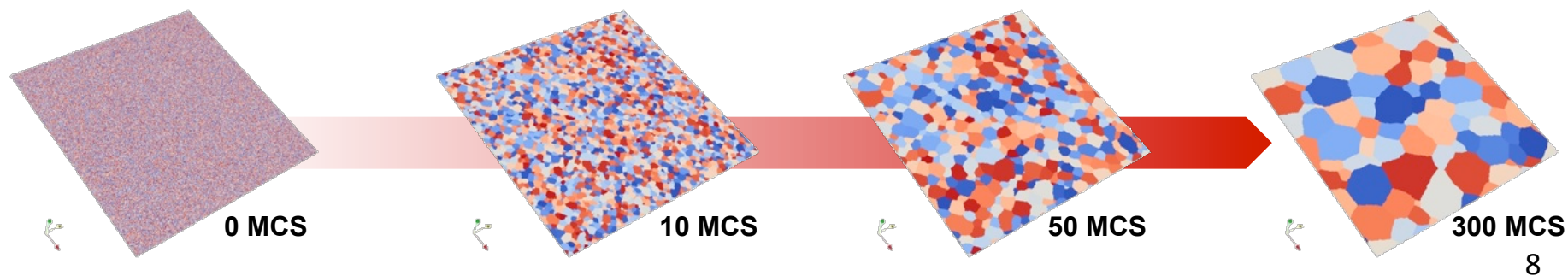


kMC for Grain Growth



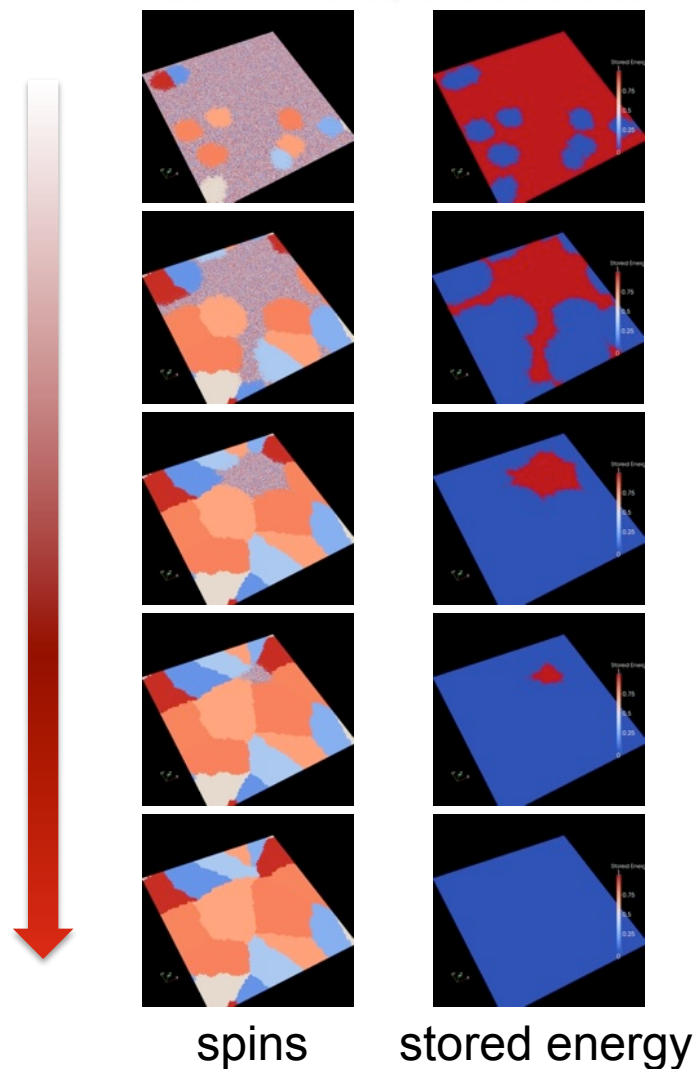
$$E_{GG} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^{neigh} [1 - \delta(q_i, q_j)]$$

$$P = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T_S}\right) & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases}$$



C.A. for Recrystallization

Binary Energy Case [$e = 1$ or 0]
2Dimensional, Site Saturated



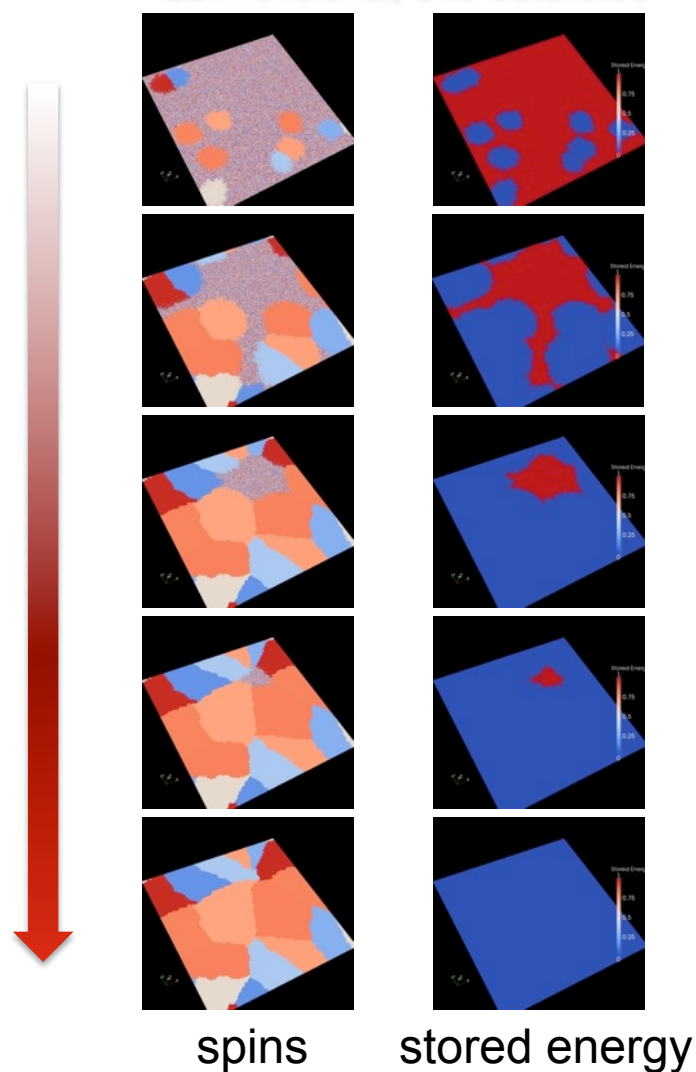
$$\text{if } \Omega_i < \Omega_j^{\text{initial}} \begin{cases} \Omega_j = \Omega_i \\ \text{spin}_j = \text{spin}_i \end{cases}$$

Although the CA approach is entirely stored energy dependent, changes of spin accompany all recrystallization events. Should a neighboring grain possess a higher energy, under recrystallization, that grain will inherit both the lower stored energy and spin of the adjacent grain

$$\Delta E_{i,RC} = \Omega_i^{\text{final}} - \Omega_i^{\text{initial}} \quad P = \begin{cases} 0 & \text{if } \Delta E > 0 \\ \frac{|\Delta E_{i,RC}|}{\Omega^{\text{MAX}}} & \text{if } \Delta E \leq 0 \end{cases}$$

C.A. for Recrystallization

Binary Energy Case [$e = 1$ or 0]
2Dimensional, Site Saturated

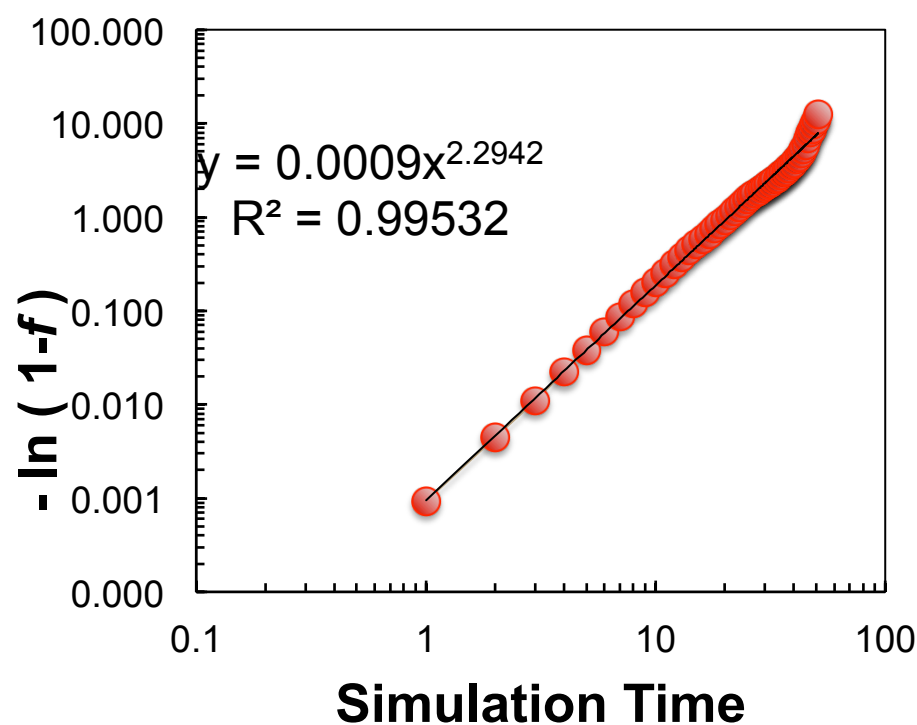


$Spins = 100$

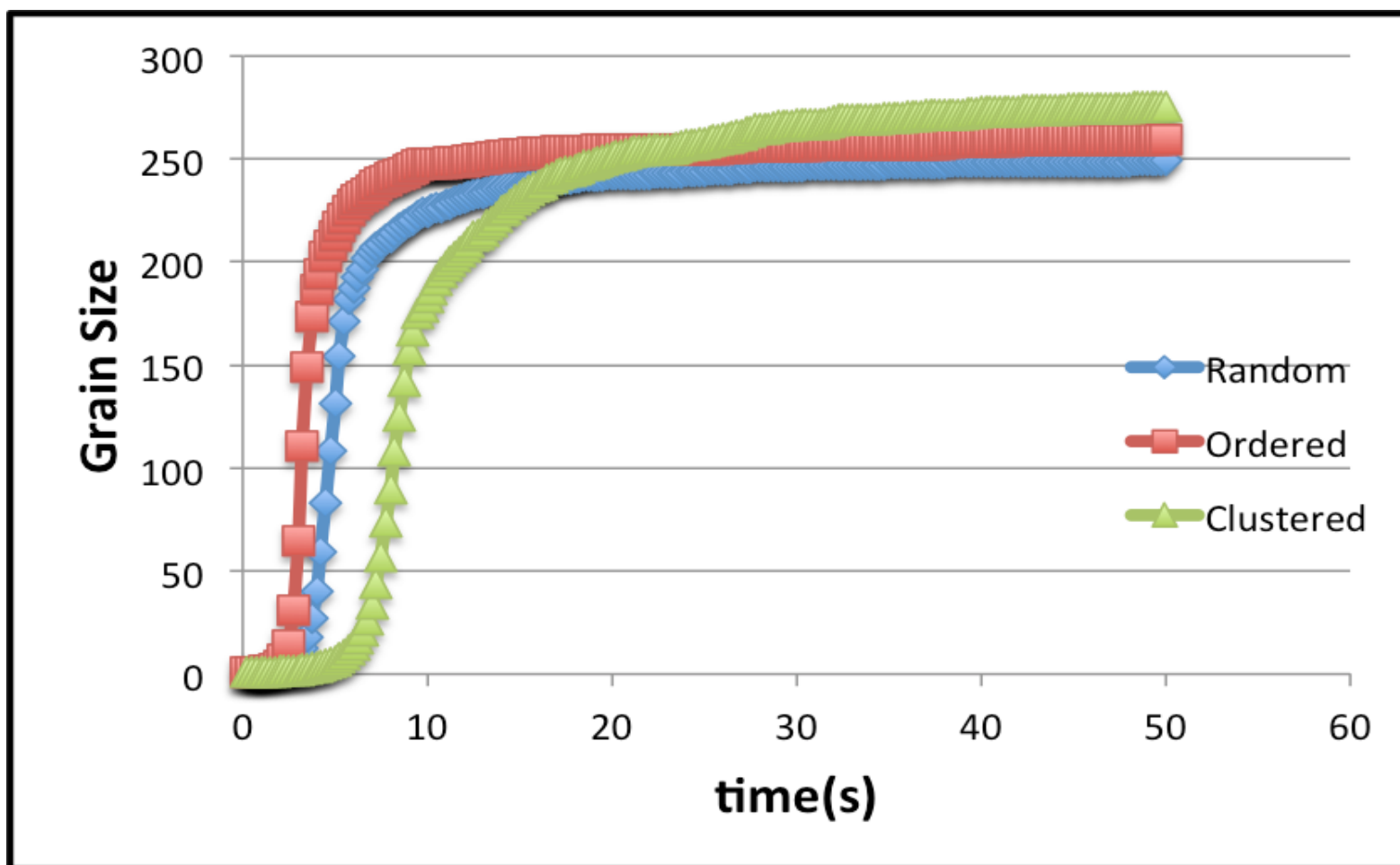
$Total Sites = 250\,000$

$Total N_{accepted} = 247\,418$

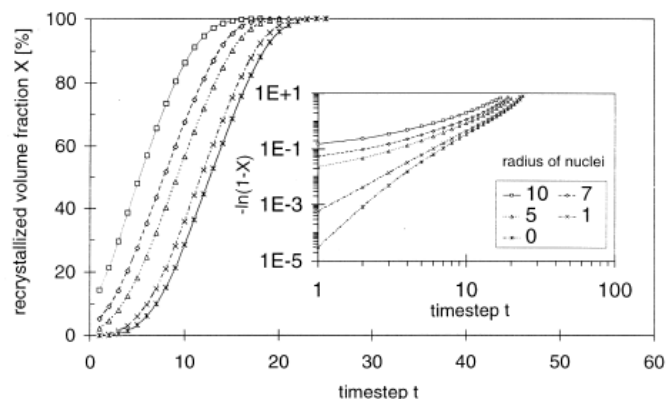
$$(1 - f) = \frac{(Total N_{accepted} - N_{accepted})}{Total N_{accepted}}$$



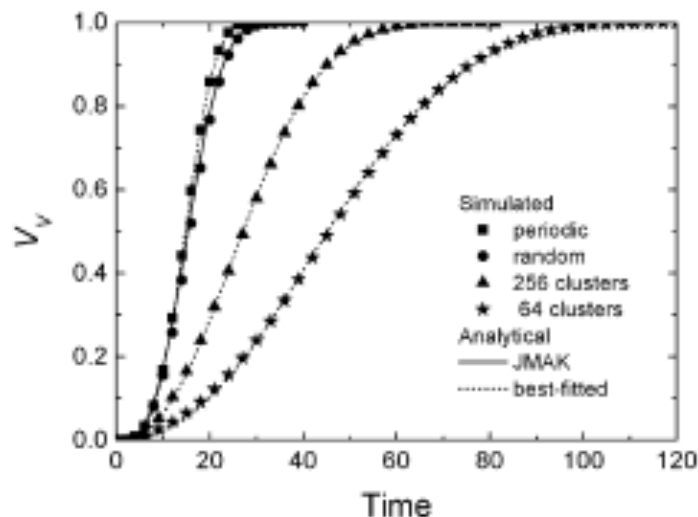
Grain Size



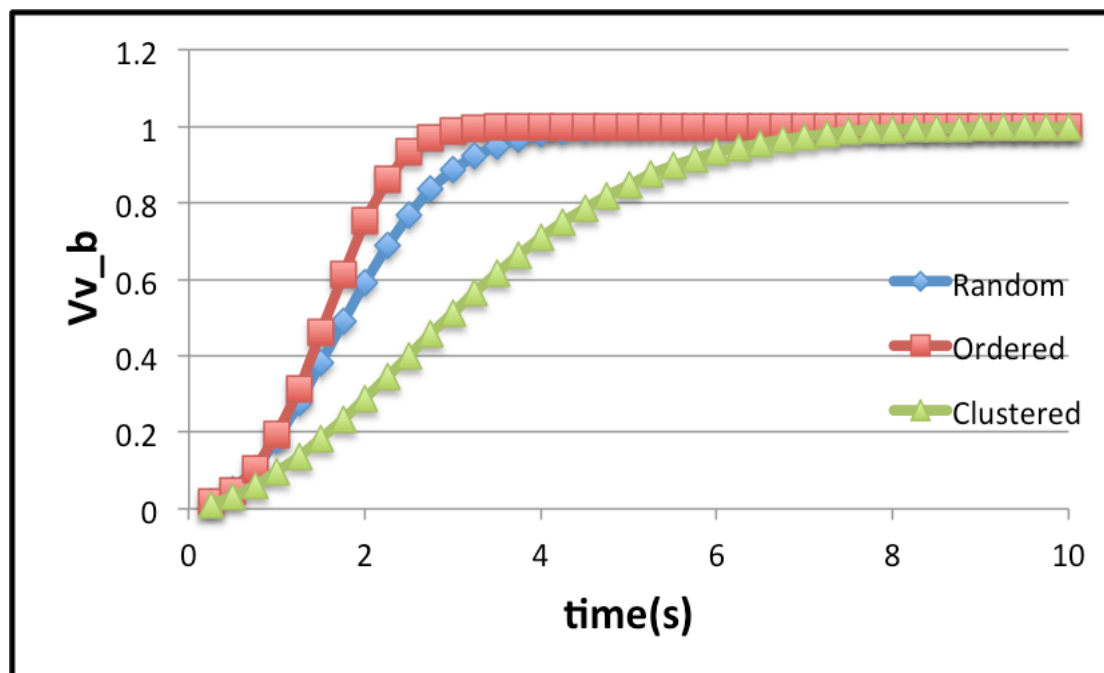
Volume Fraction



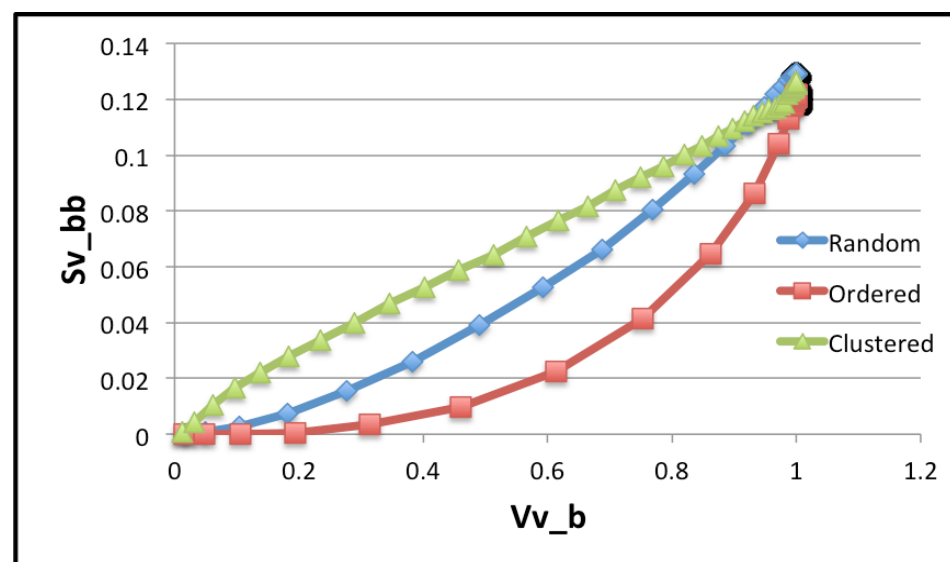
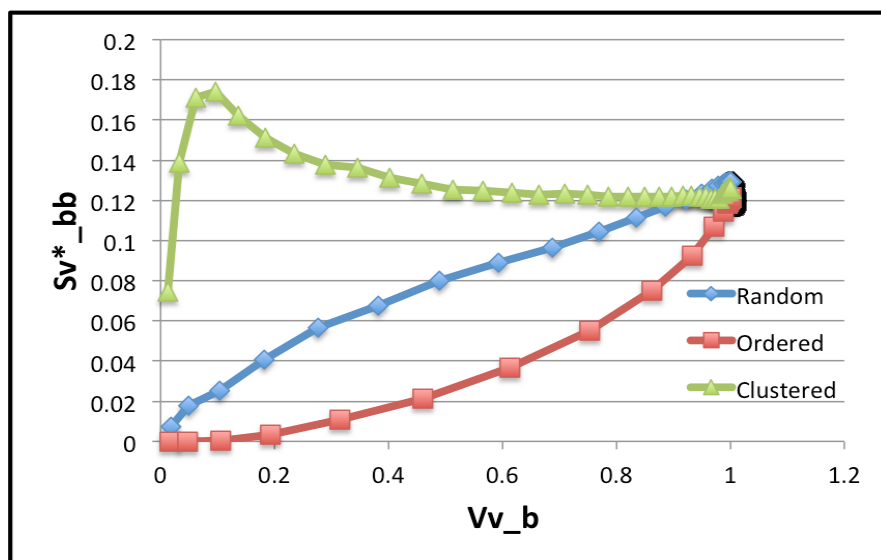
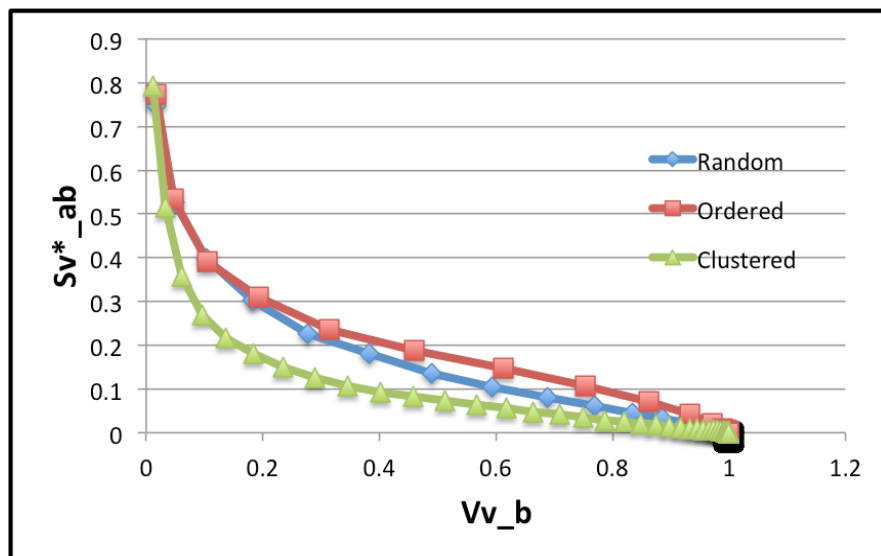
Marx et al: *Acta Mat.*, 1999, vol. 47
pp. 1219-1230.



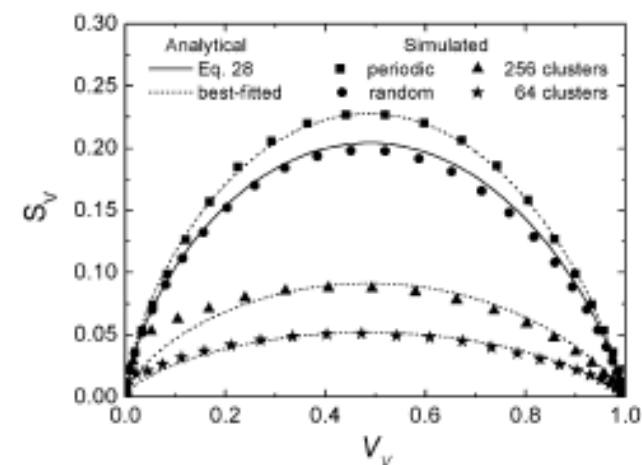
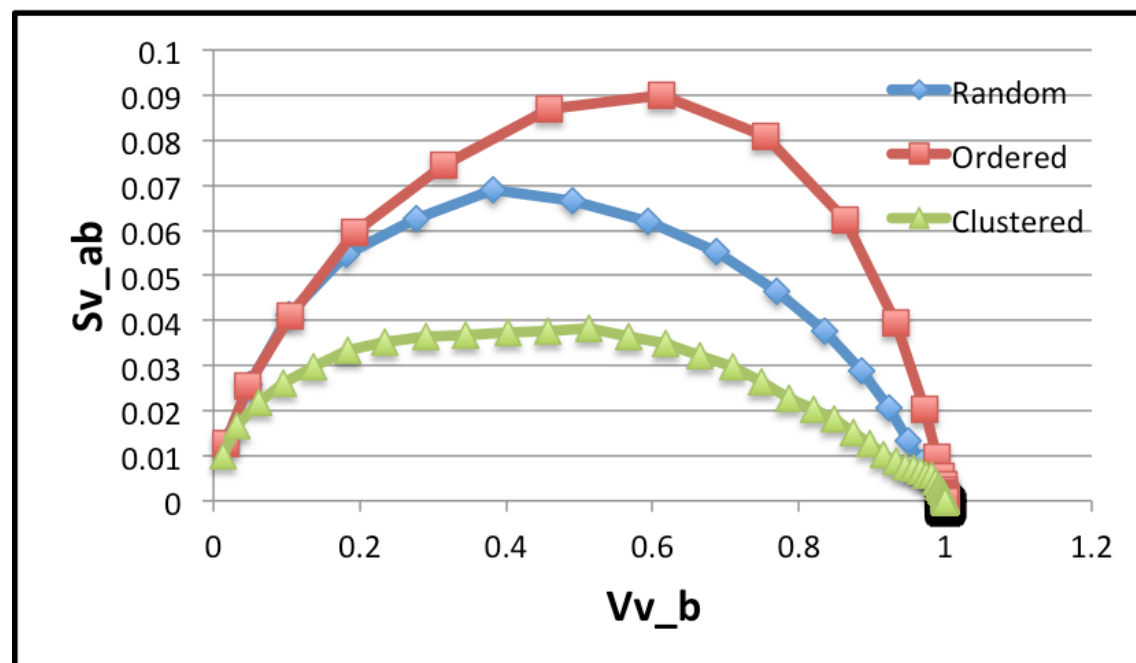
P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro:
Acta Mat., 2007, vol. 55 pp. 4339-48.



Interfacial Surface Area I

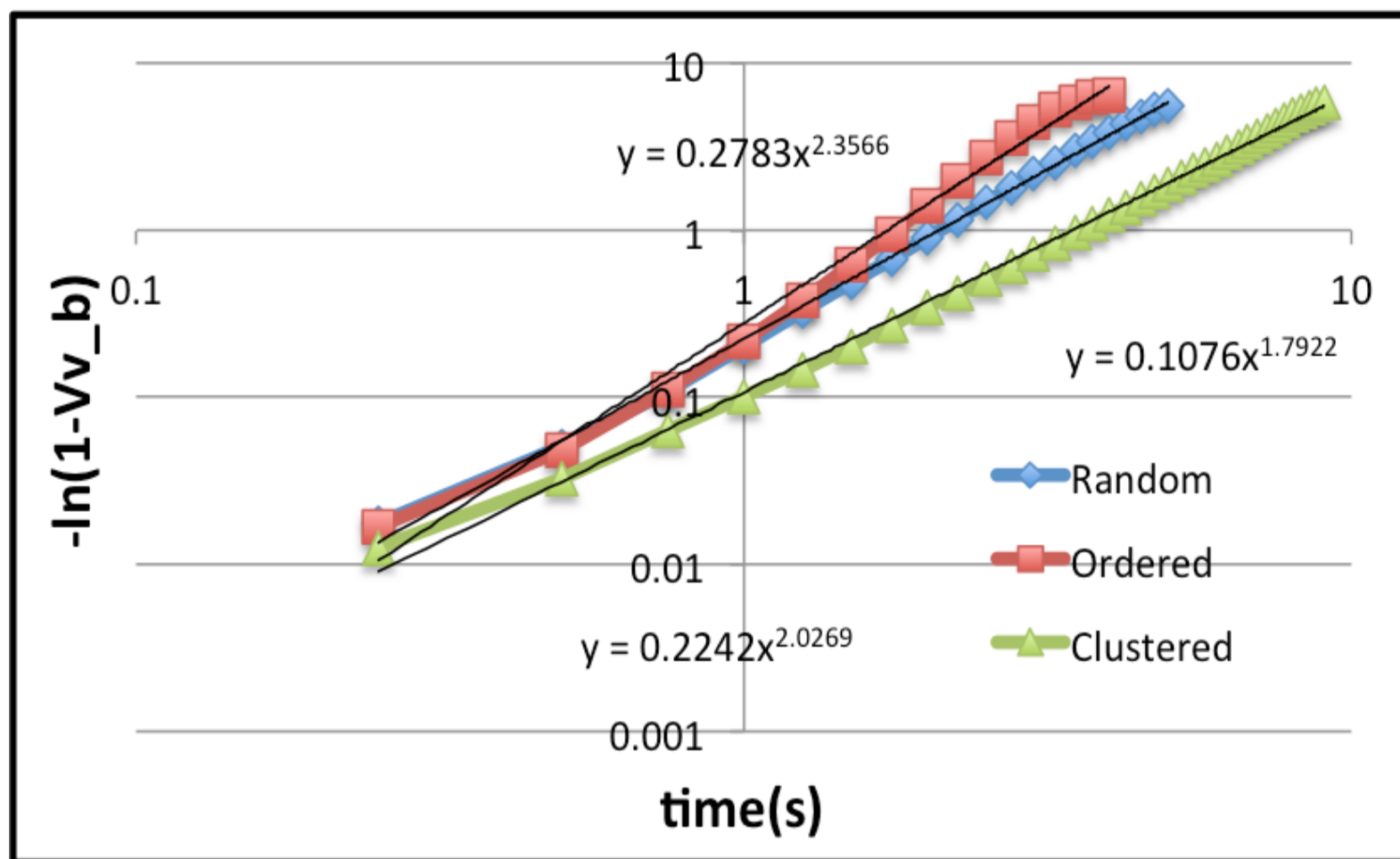


Interfacial Surface Area II



P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro:
Acta Mat., 2007, vol. 55 pp. 4339-48.

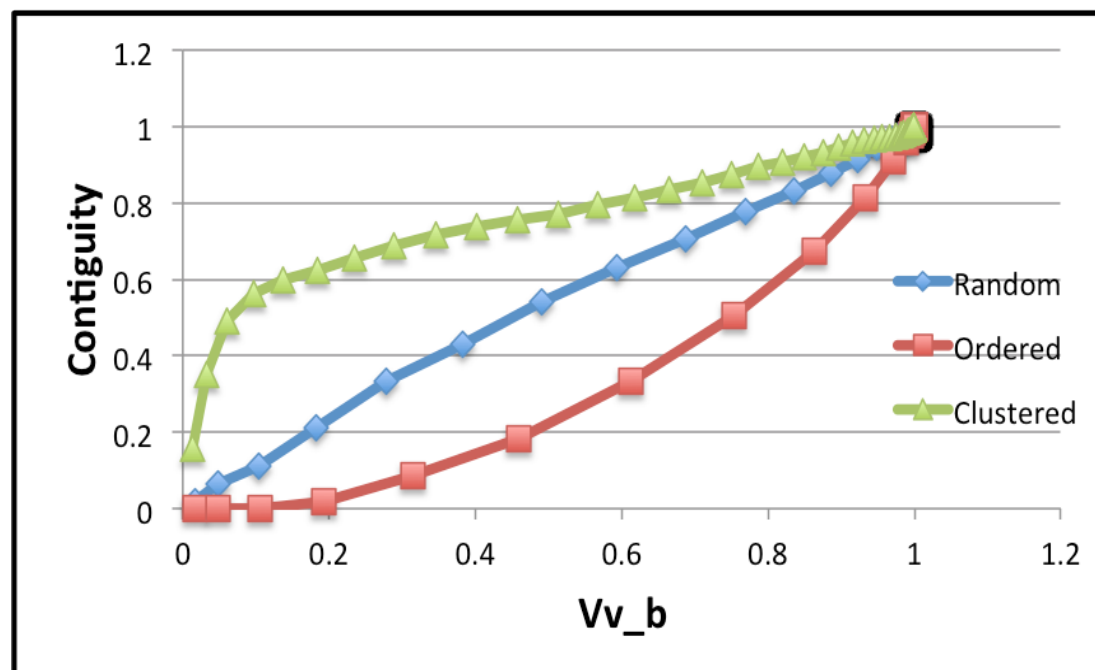
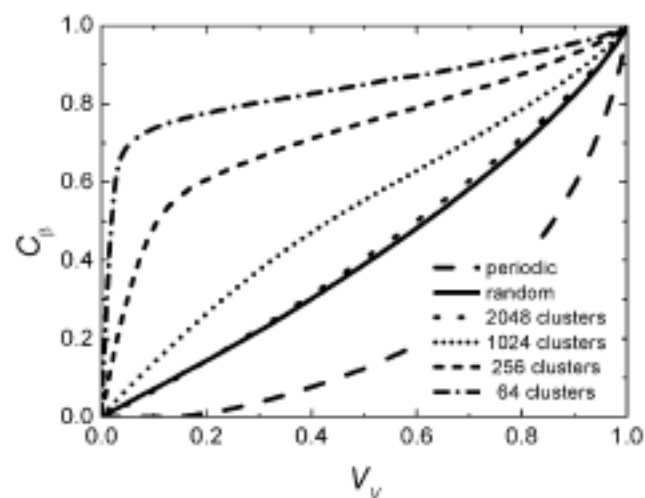
KJMA Exponent



Contiguity

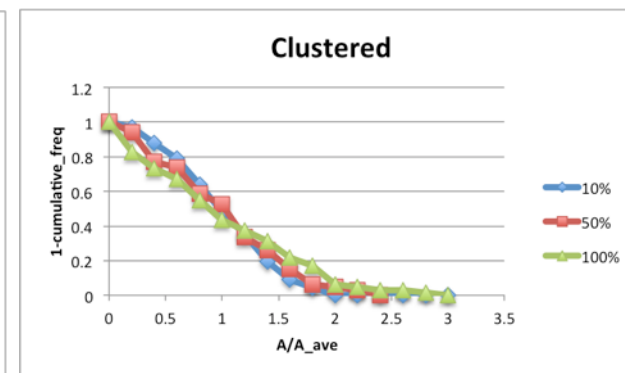
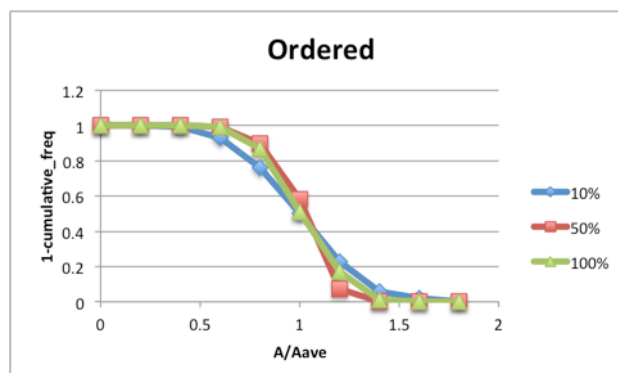
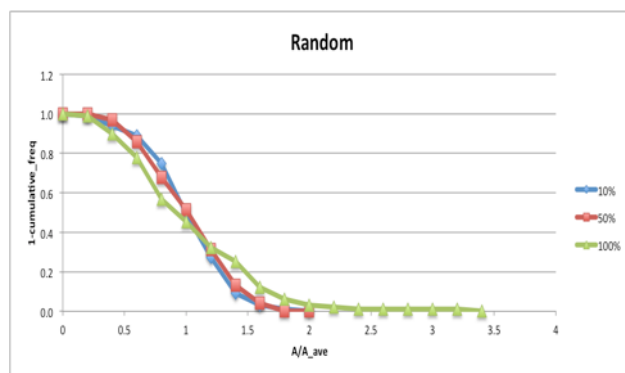
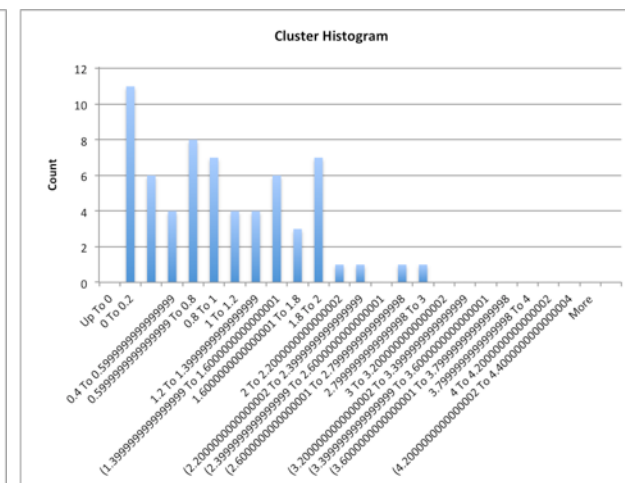
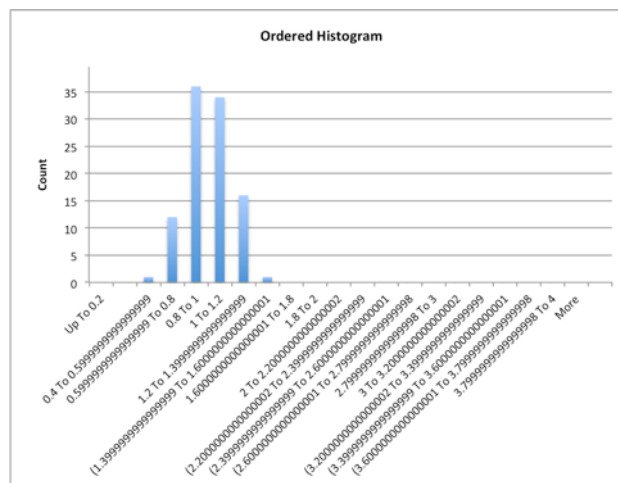
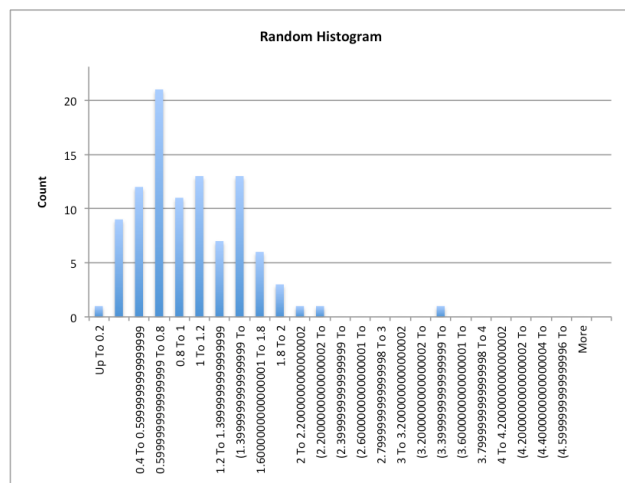
R. Vandermeer: *Acta Mat.*, 2005, vol. 53 pp. 1449-1457.

$$C_{\alpha\alpha} = \frac{2(S_v)_{\alpha\alpha}}{2(S_v)_{\alpha\alpha} + (S_v)_{\alpha\beta}}$$



P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro:
Acta Mat., 2007, vol. 55 pp. 4339-48.

Distributions

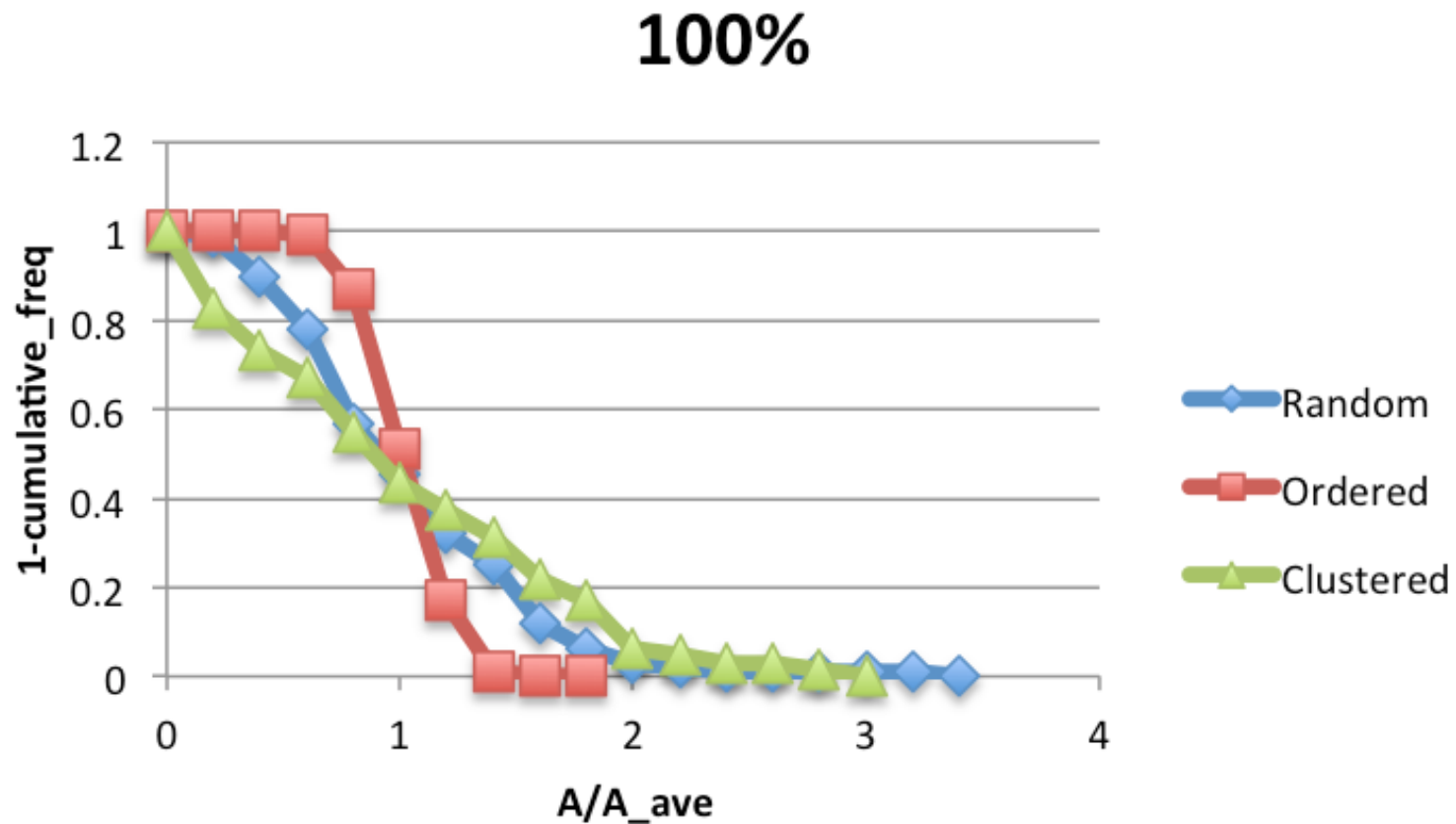


	10%	50%	100%
Mean	244.6060606	1273.767677	2525.252525
Stand. Dev.	80.56177984	436.3379571	1396.013233
C.V.	0.329353163	0.34255694	0.55282124

	10%	50%	100%
Mean	260.07	1234.53	2499.91
Stand. Dev.	68.55717293	177.588985	457.5953418
C.V.	0.263610462	0.143851494	0.183044726

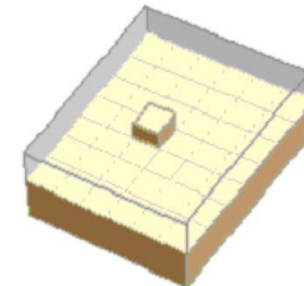
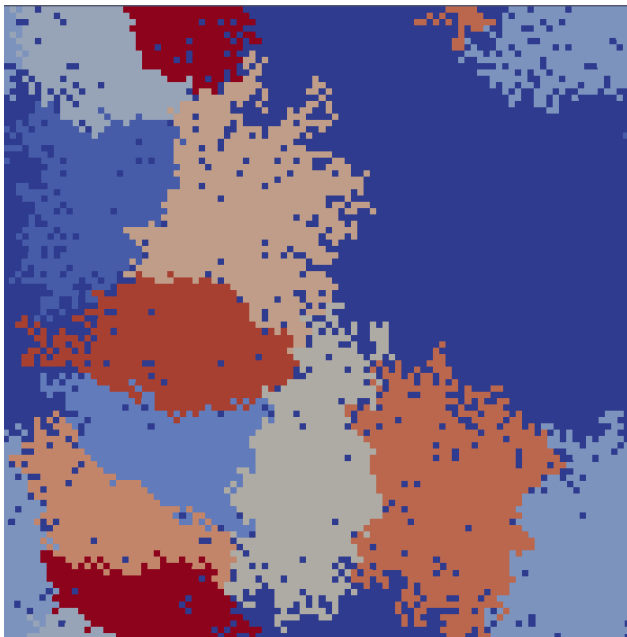
	10%	50%	100%
Mean	401.9545455	1935.184615	3906.25
Stand. Dev.	185.06119	1091.347045	2778.123667
C.V.	0.460403277	0.563949835	0.711199659

Cumulative Frequency Distributions

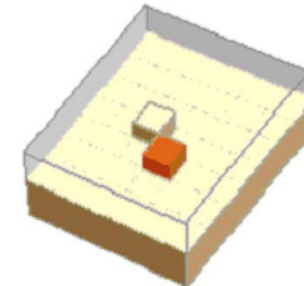


Future Work

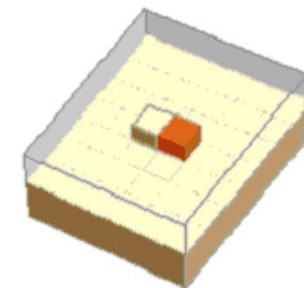
- Future work will focus on extending the simulation framework into three-dimensions
- Initial work shows enhanced surface roughness when employing three dimensions. This artifact has been denoted as “the model-lattice effect” by other investigators.



(a)



(b)



(c)

O. M. Ivasishin, et al., Mater. Sci. Eng. A, 2006, vol. 433 pp. 216-232.

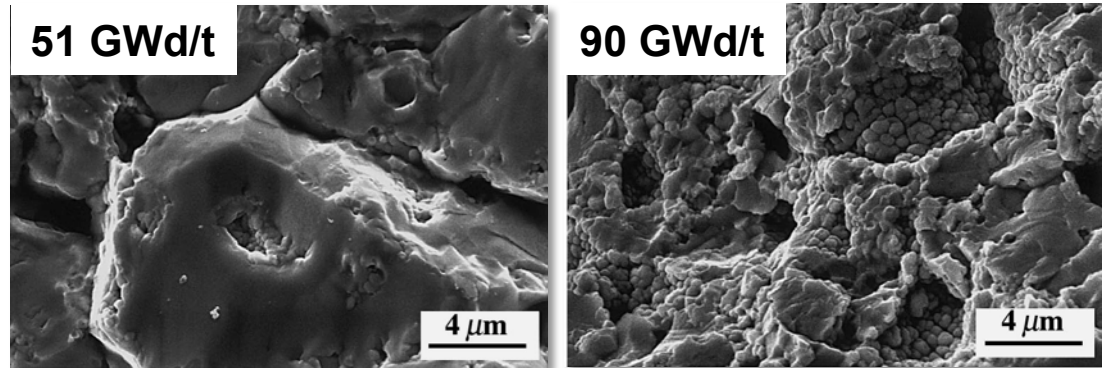
Summary

- The kMC-C.A. hybrid model reliably mimics static recrystallization behavior in a 2D model
- A readily deployable methodology for tracking microstructural evolution has been advanced to include inter- and intra-phase interfacial surface areas, KJMA exponents, contiguity and size distributions in discretized lattice microstructures
- Tracked features show agreement with trends previously identified by Marx et al., Vandermeer and Rios et al.

Questions

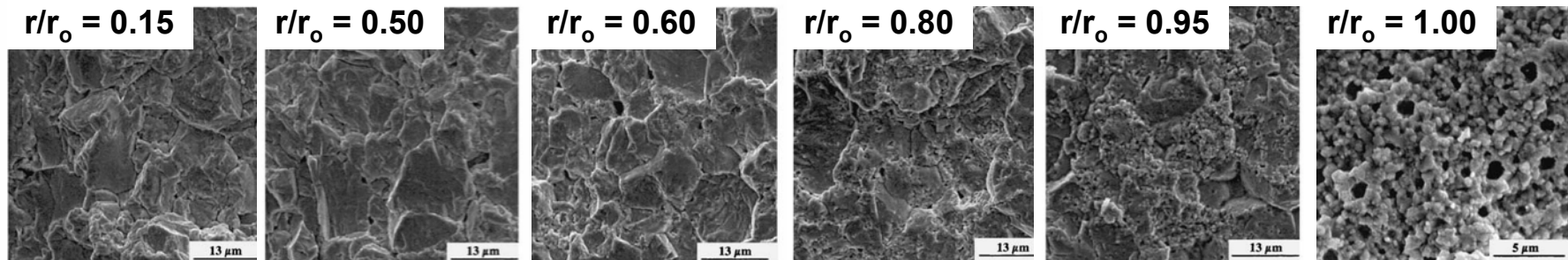
High Burn-Up Structure I

- Rim structure is a function of burn-up
- Low burn-up, original grain structure
- With ^{239}Pu formation, recrystallization occurs where enrichment is most pronounced



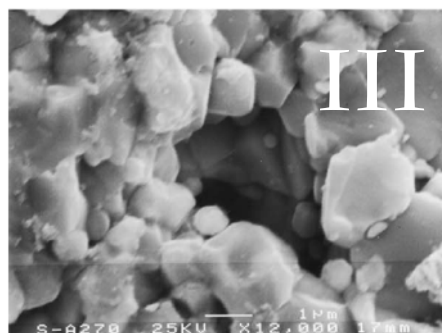
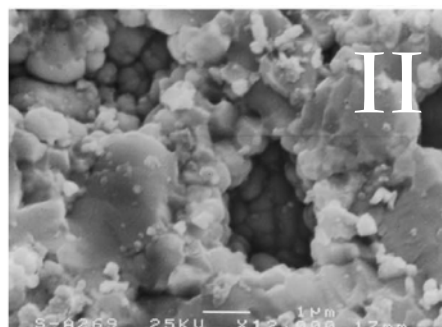
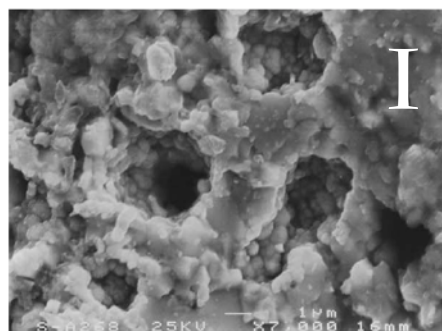
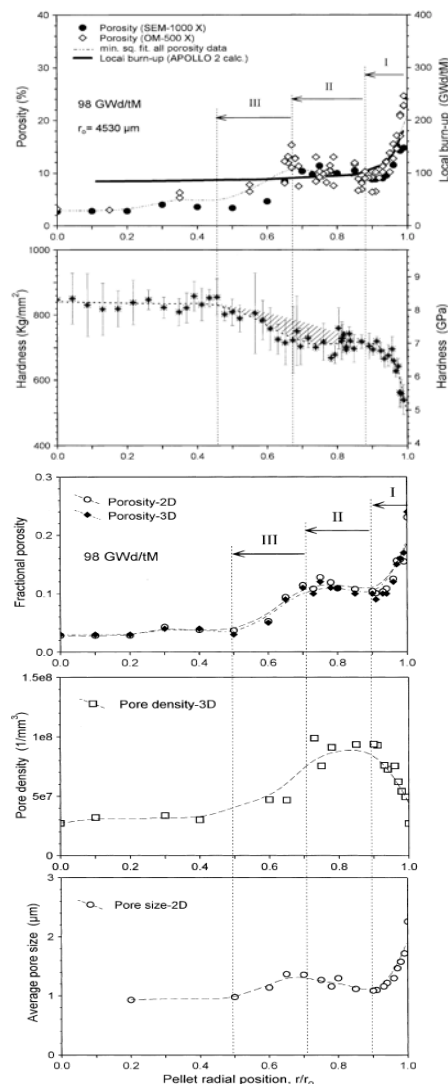
Une, et. al, JNM vol. 288, 2001

- Since burn-up correlates with radial position recrystallization is largely absent as r/r_o decreases



Manzel & Walker, JNM vol. 301, 2002

High Burn-Up Structure II



- Understanding the rim effect is important
 - Effects fuel performance (thermal conductivity, fission product distributions, ...)
 - Effects mechanical properties during storage and transportation
 - Modifies the separation processes for fuel recycling.
- Various aspects of the evolutionary process are analogous to metallic systems undergoing dynamic recrystallization.