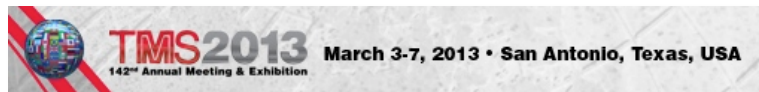
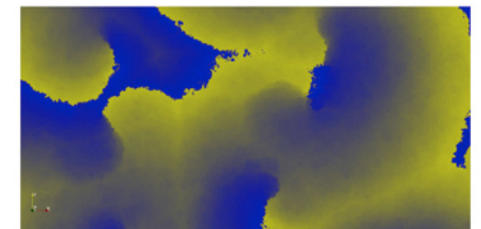
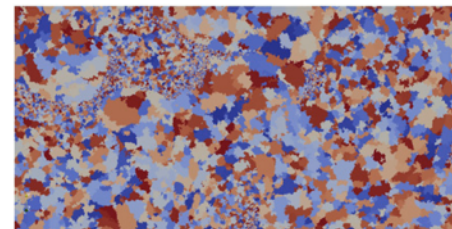
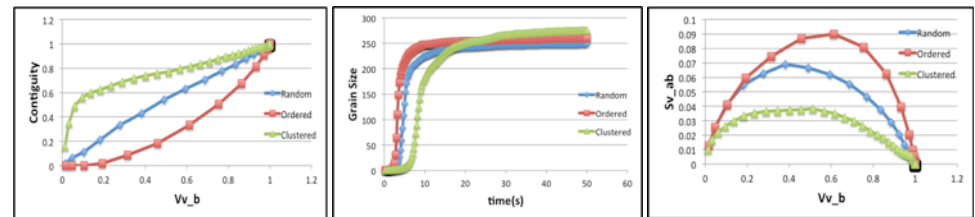


Parametric Study of a Potts Recrystallization Model

D. J. Rule, J. Madison, V. Tikare

*Exceptional service
in the national interest*



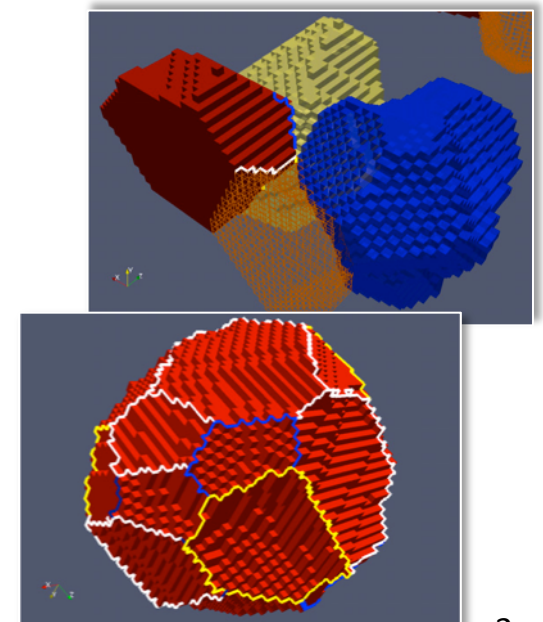
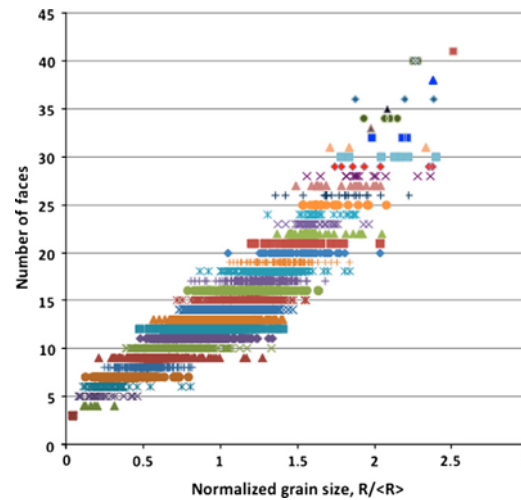
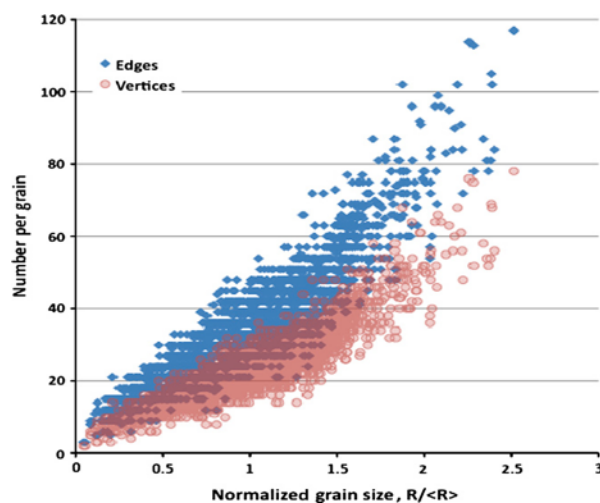
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND No. 2011-XXXXP.

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
 - XXX -- Cahn-Hagel Growth Rate – XXX
 - 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

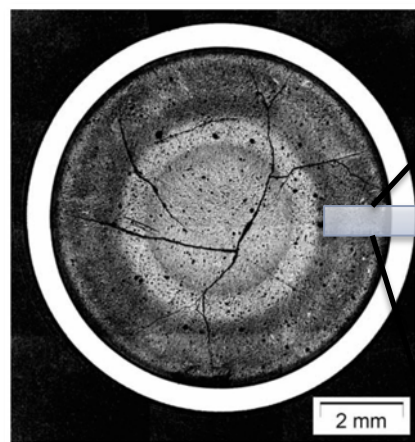


❖ Z. Sun, V. Tikare, B. R. Patterson and A. P. Sprague: *Comp. Mat. Sci.*, 2012, vol. 55 pp. 329-36.

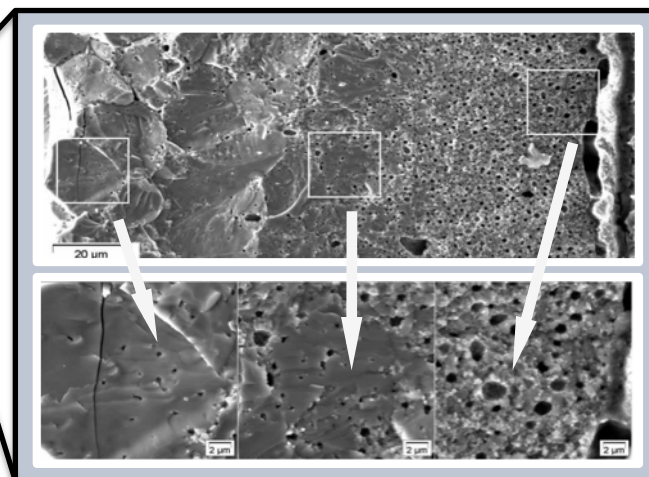
Background II

- 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
Noirot, et. al *NE&T*, vol. 41 2009



RESULT

Tremendous Variation In Microstructure

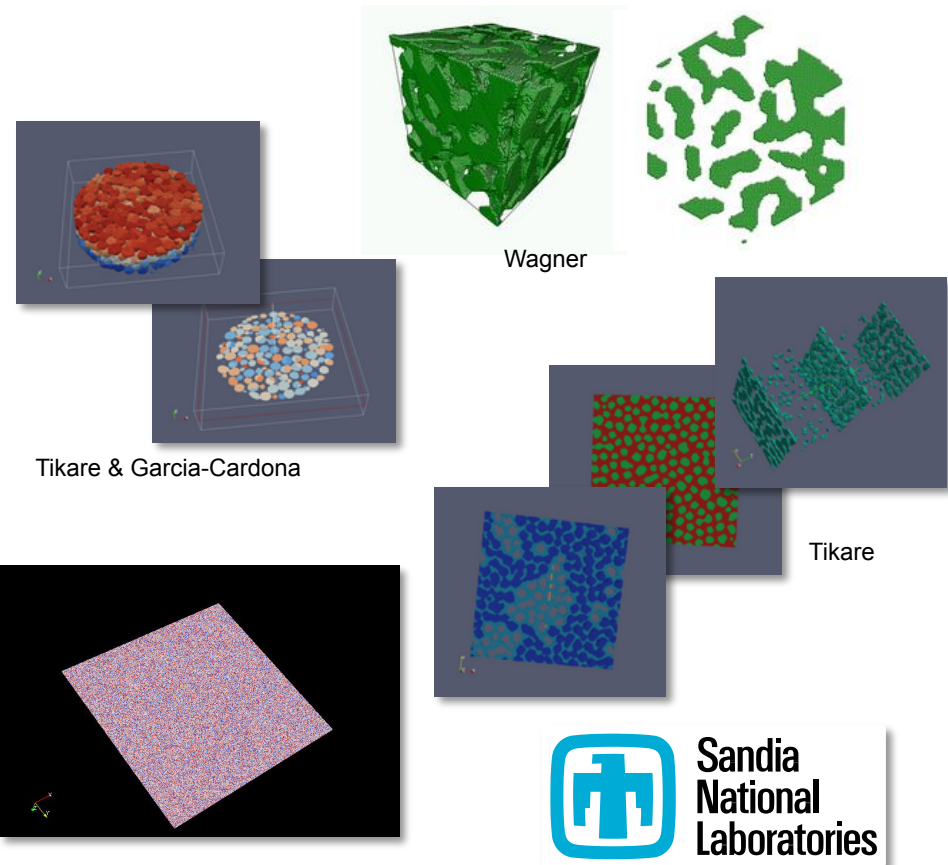
1. Grain size
2. Porosity
3. Percolation
3. Composition
4. Hardness

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



<http://www.cs.sandia.gov/~sjplimp/spparks.html>

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.

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[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.

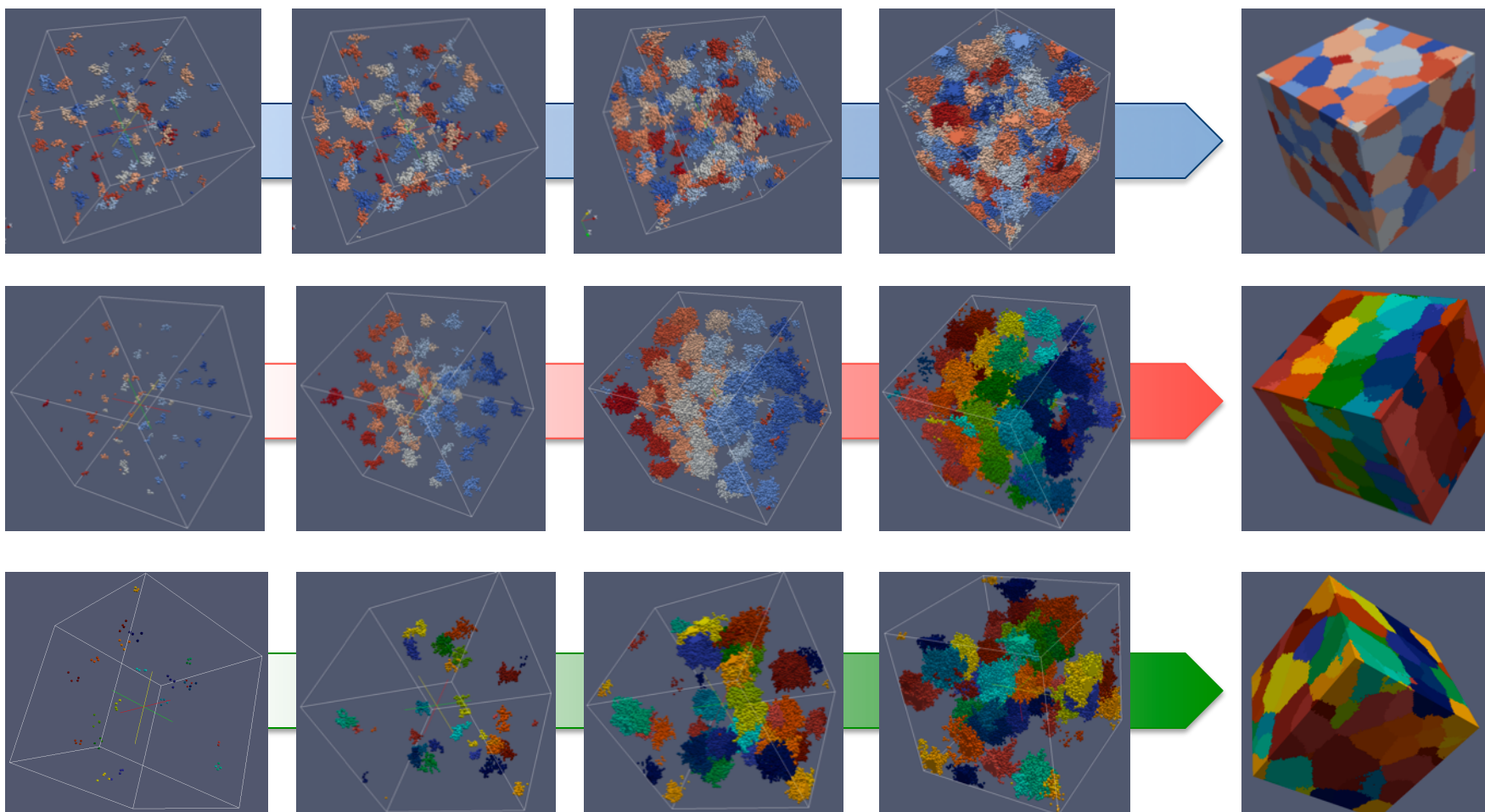
[38] D. Raabe, Cellular, Lattice Gas, and Boltzmann Automata, in: D. Raabe, F. Roters, F. Barlat, L.-Q. Chen (Eds.) Continuum Scale Simulation of Engineering Materials: Fundamentals-Microstructures-Process Applications, Wiley-VCH, Strauss GmbH, 2004, pp. 57-76.

[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.

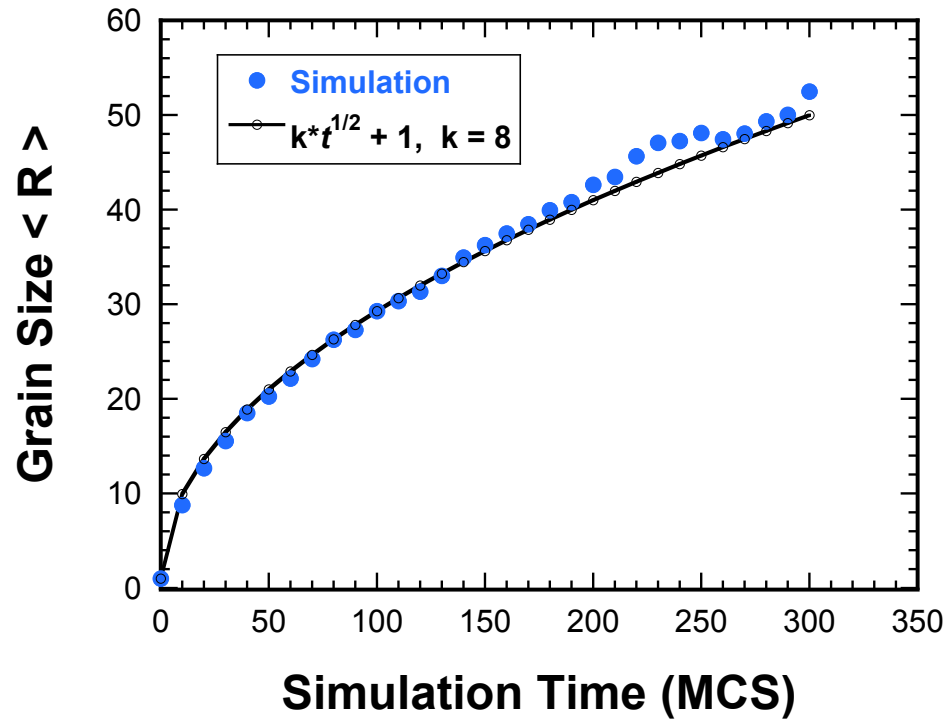
[40] D. Raabe, Mesoscale Simulation of Recrystallization Textures and Microstructures, Advanced Engineering Materials, 3 (2001) 745-752.

Nuclei Instantiation

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

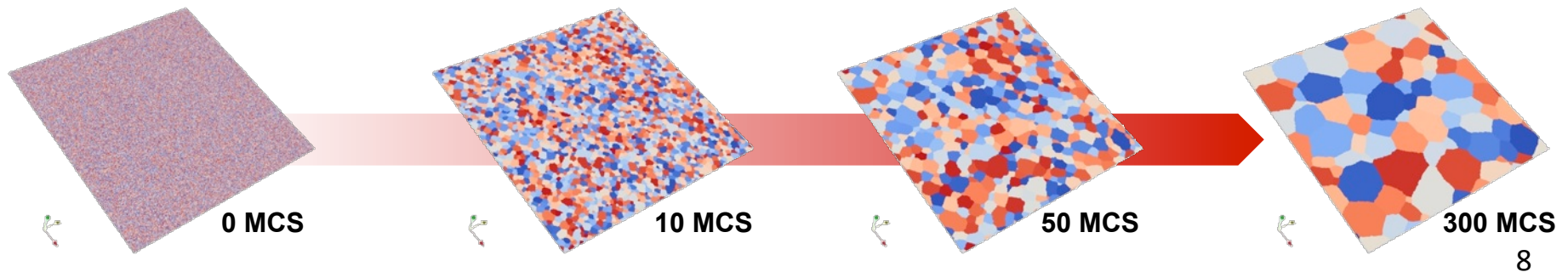


kMCMC for Grain Growth



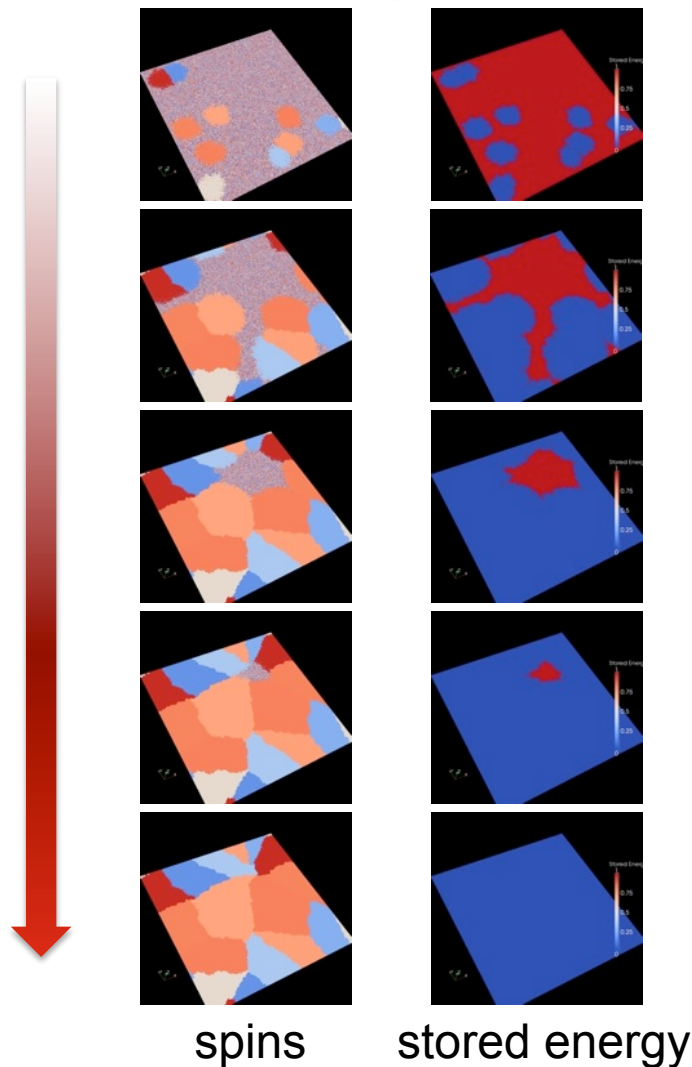
$$E_{GG} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^{neigh} [1 - \delta(q_i, q_j)]$$

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



C.A. for Recrystallization

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



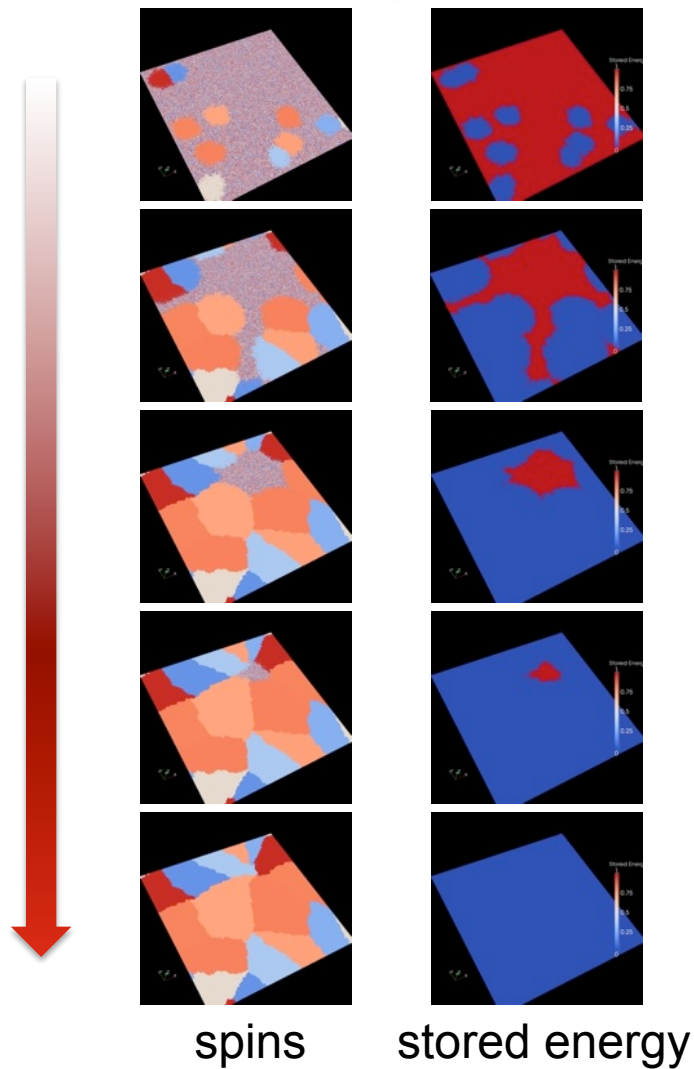
$$\text{if } \Omega_i < \Omega_j^{\text{initial}} \begin{cases} \Omega_j = \Omega_i \\ \text{spin}_j = \text{spin}_i \end{cases}$$

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

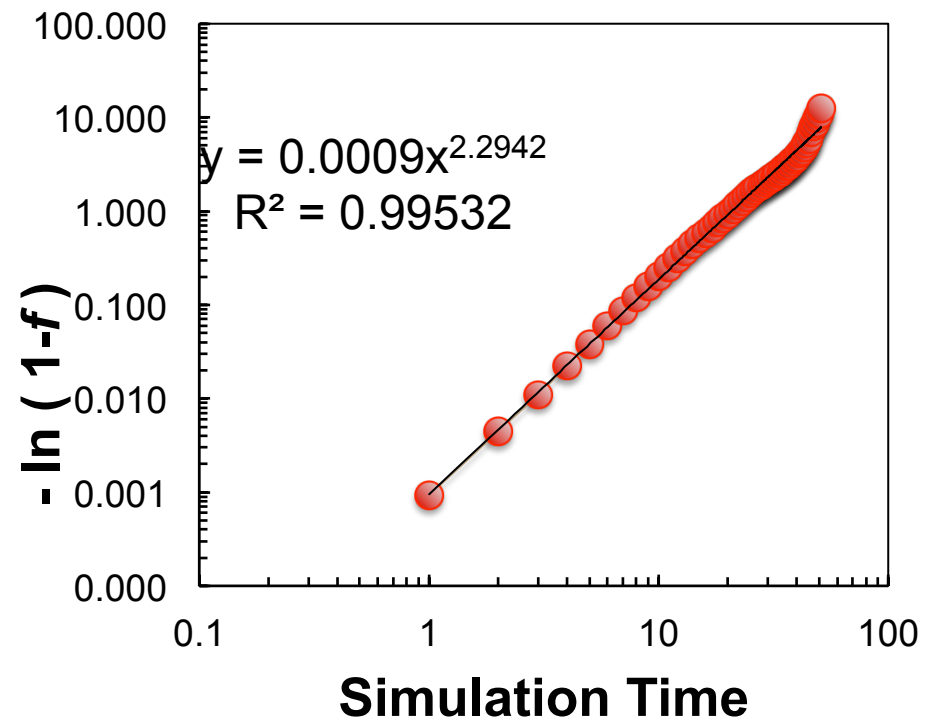


$Spins = 100$

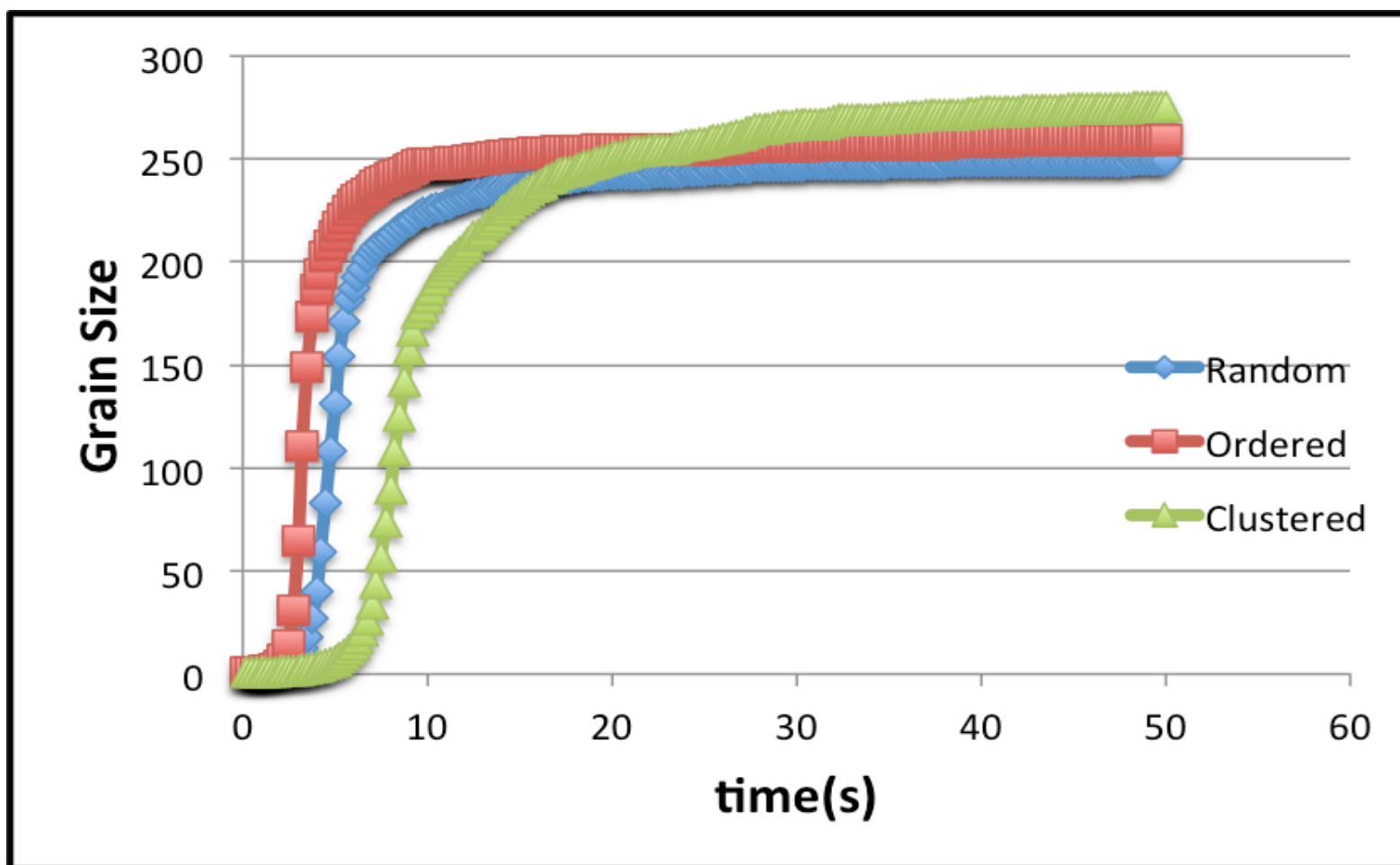
$Total Sites = 250\ 000$

$Total N_{accepted} = 247\ 418$

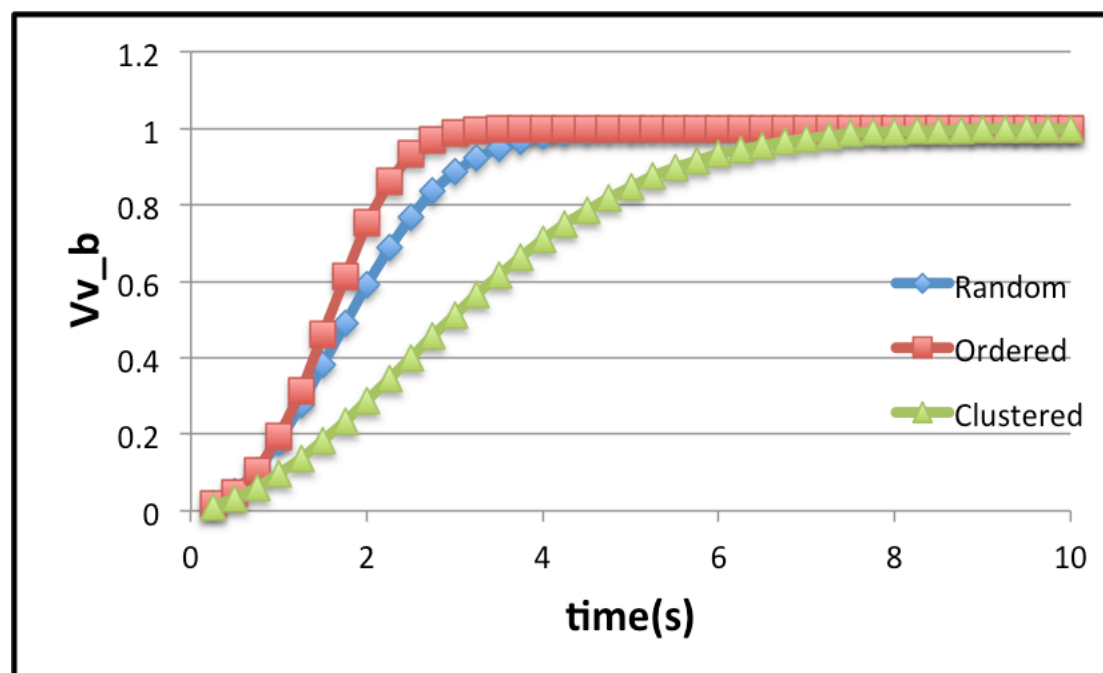
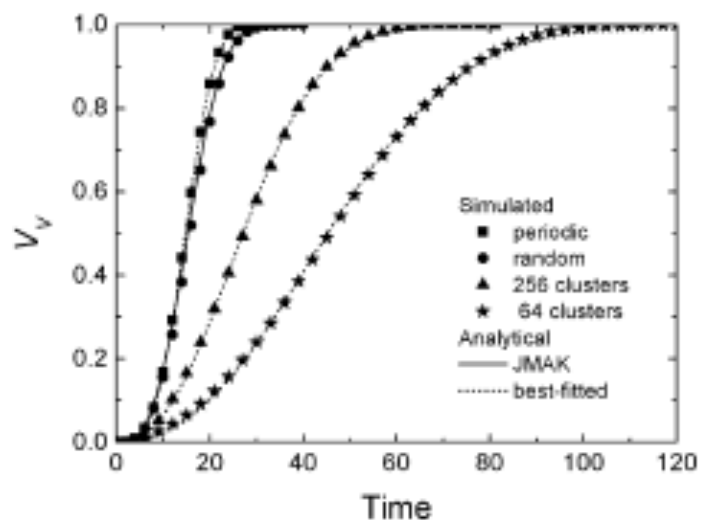
$$(1 - f) = \frac{(Total N_{accepted} - N_{accepted})}{Total N_{accepted}}$$



Grain Size

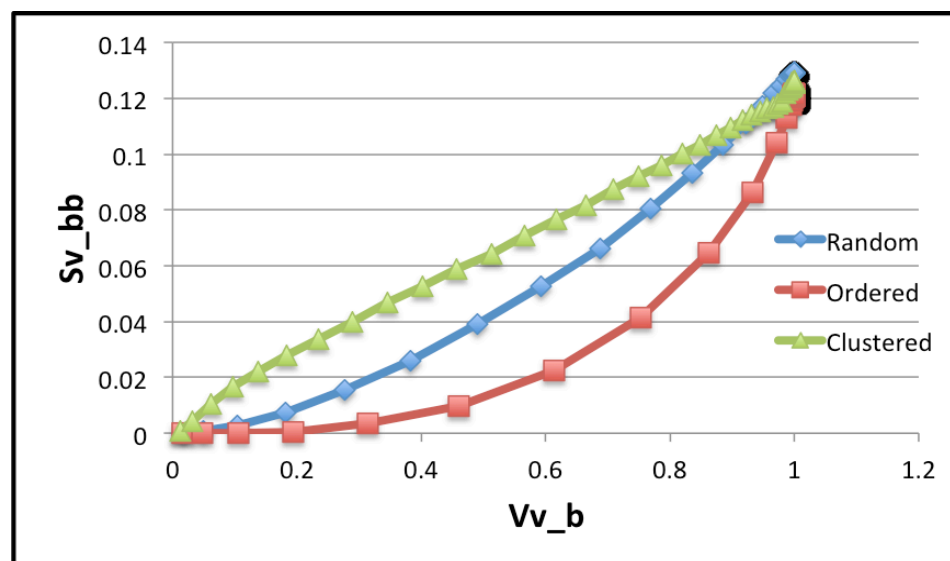
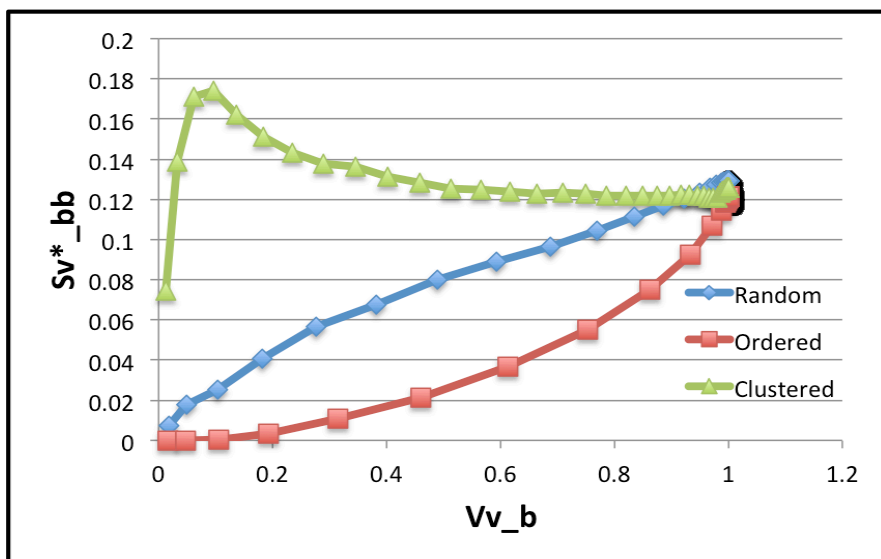
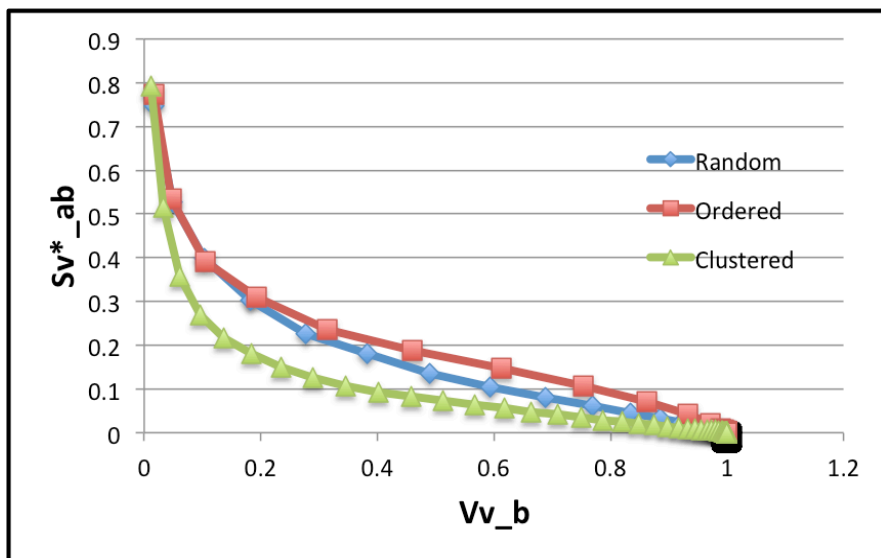


Volume Fraction

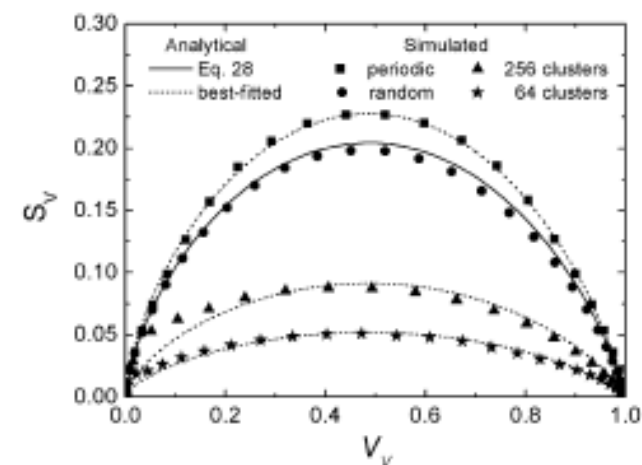
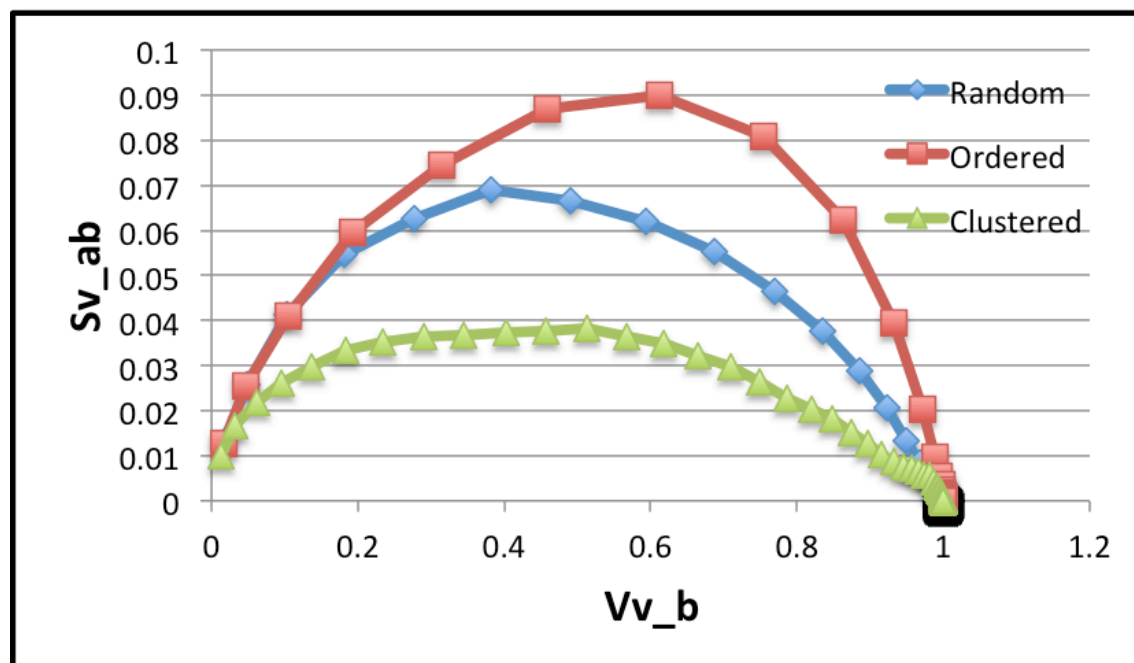


P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro:
Acta Mat., 2007, vol. 55 pp. 4339-48.

Interfacial Surface Area I

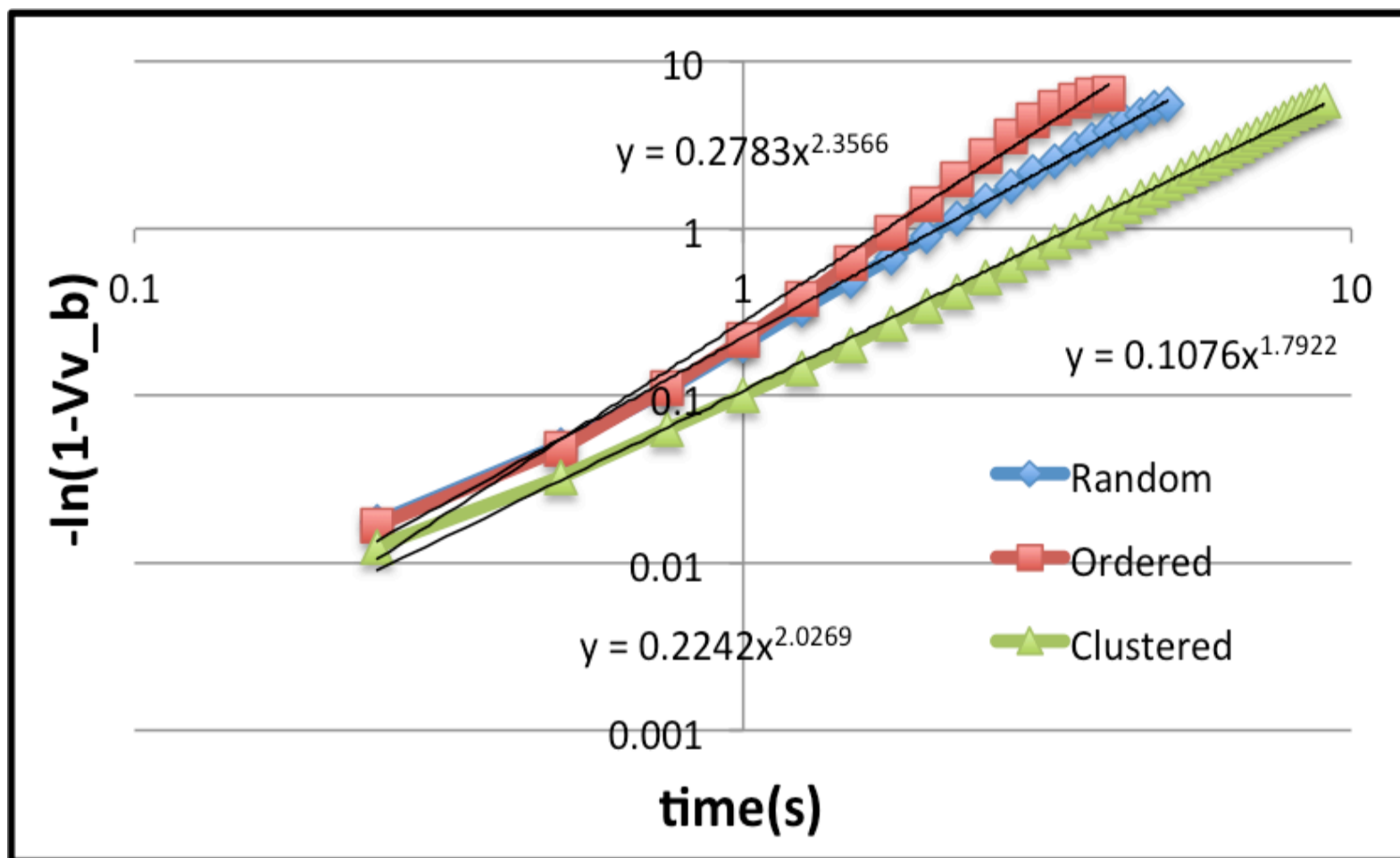


Interfacial Surface Area II

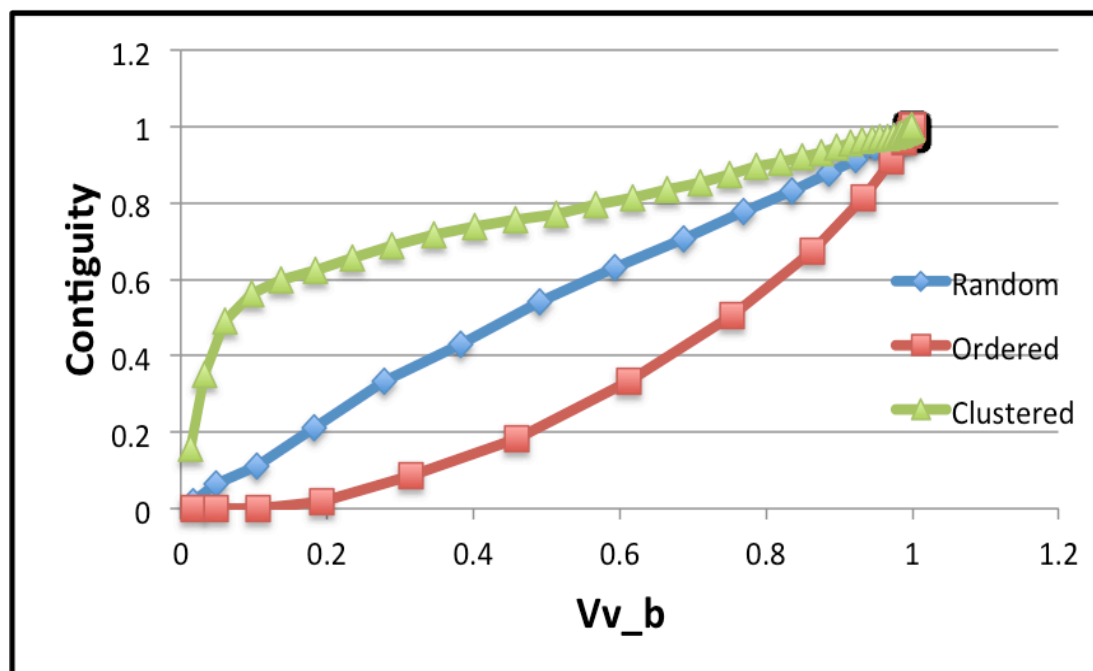
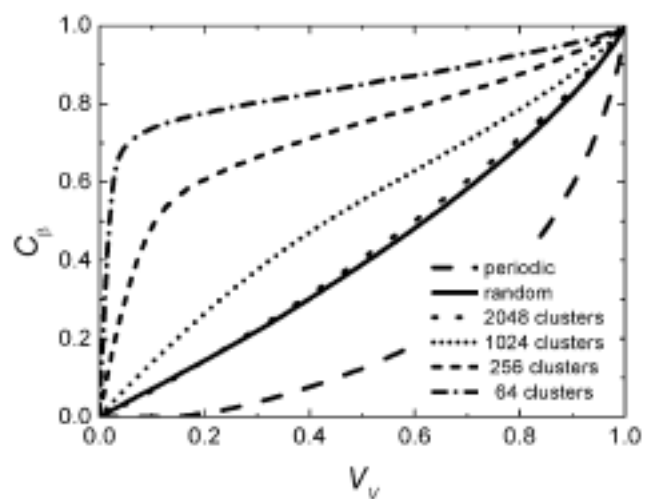


P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro:
Acta Mat., 2007, vol. 55 pp. 4339-48.

KJMA Exponent

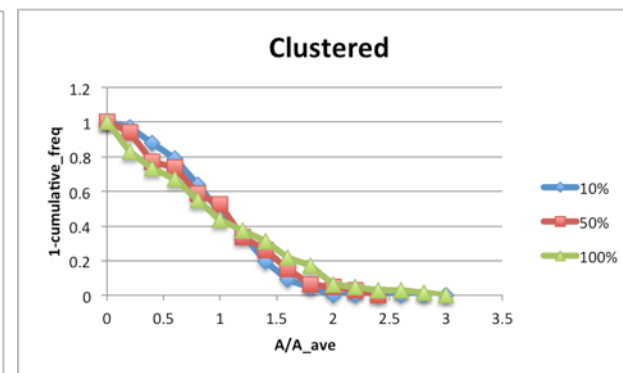
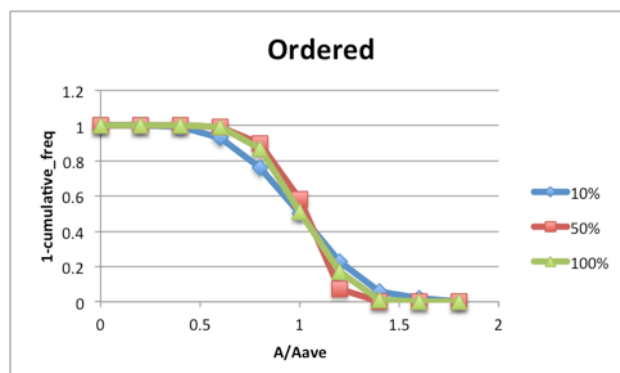
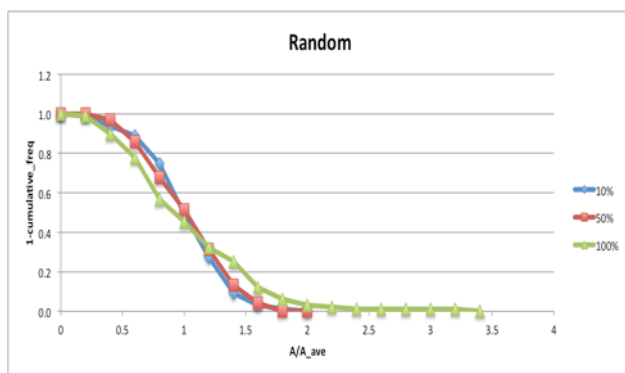
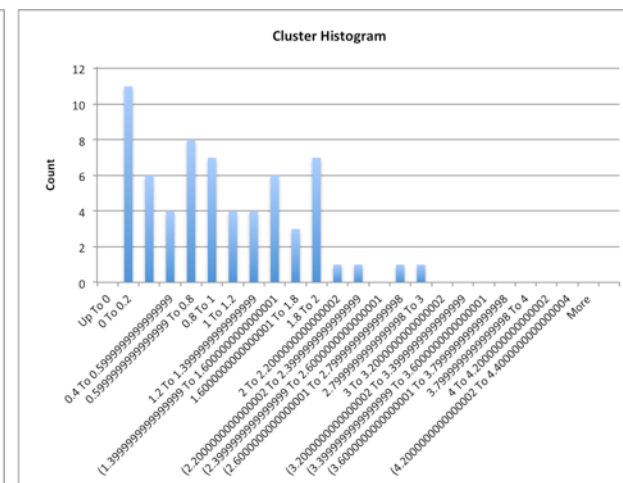
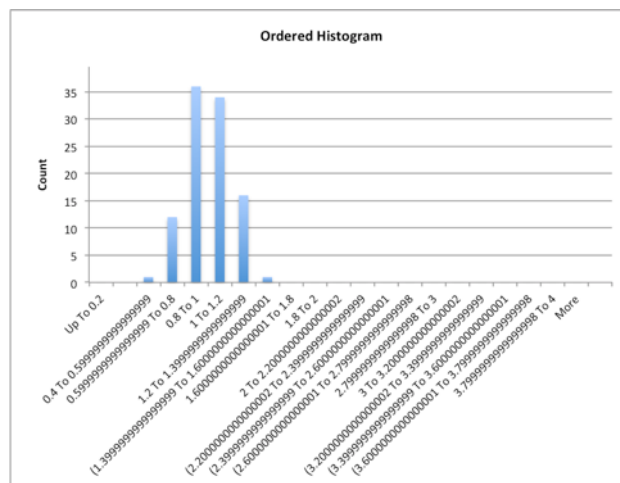
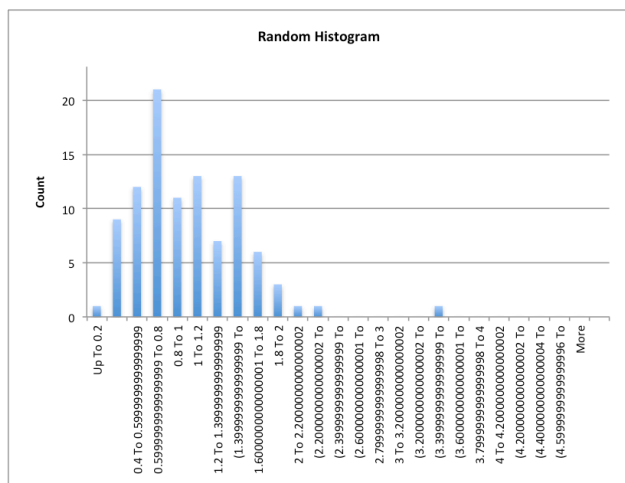


Contiguity



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



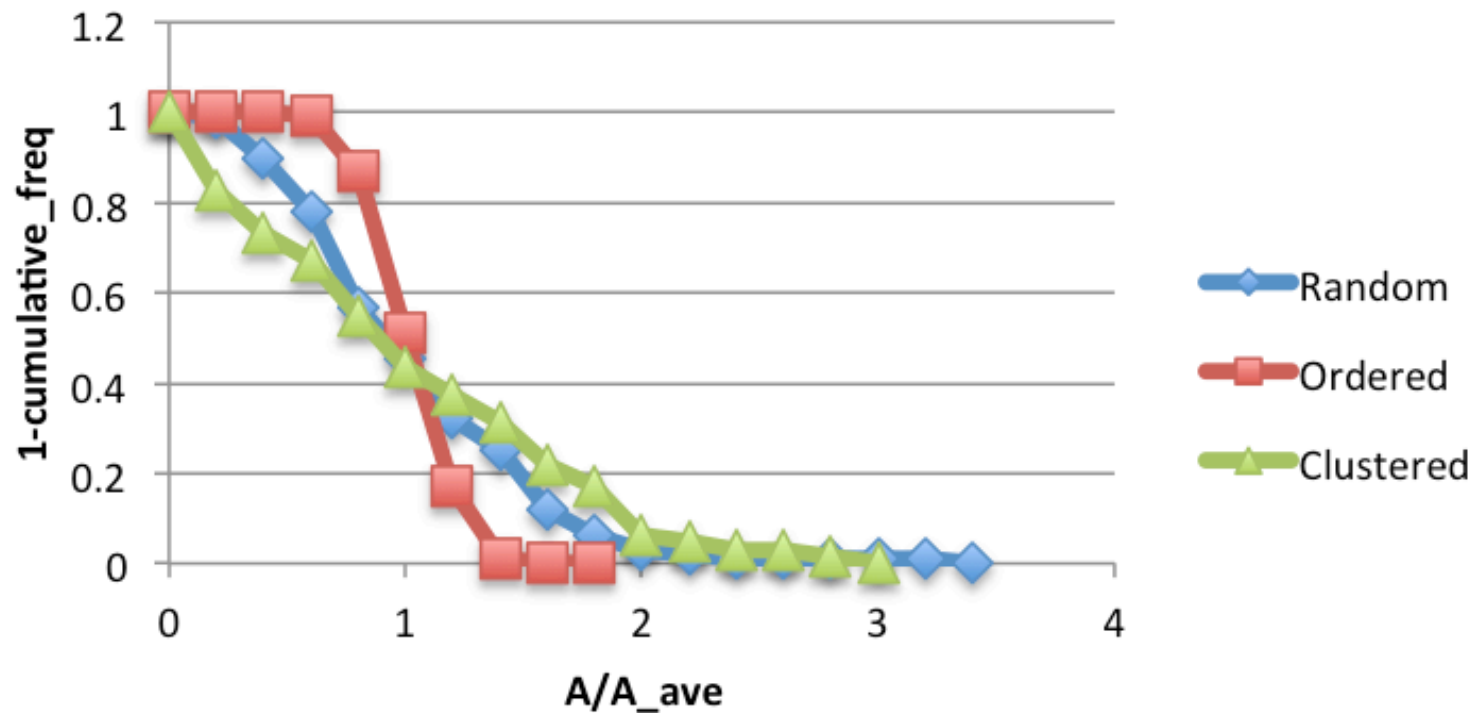
	10%	50%	100%
Mean	244.6060606	1273.767677	2525.252525
Stand. Dev.	80.56177984	436.3379571	1396.013233
C.V.	0.329353163	0.34255694	0.55282124

	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

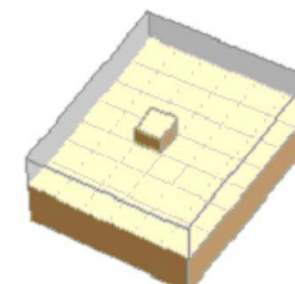
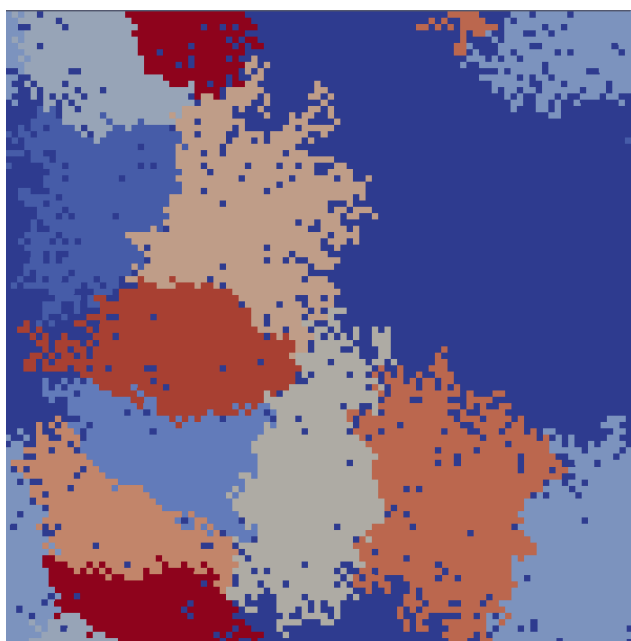
Cumulative Frequency Distributions

100%

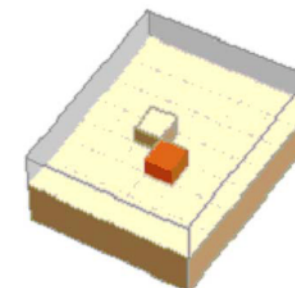


Future Work

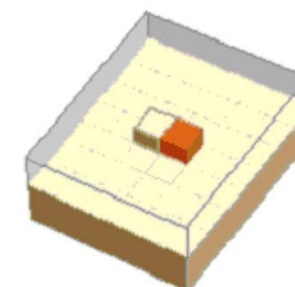
- Future work will focus on extending the simulation framework into three-dimensions
- Initial work shows enhanced surface roughness when employing three dimensions. This artifact has been denoted as “the model-lattice effect” by other investigators.



(a)



(b)



(c)

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

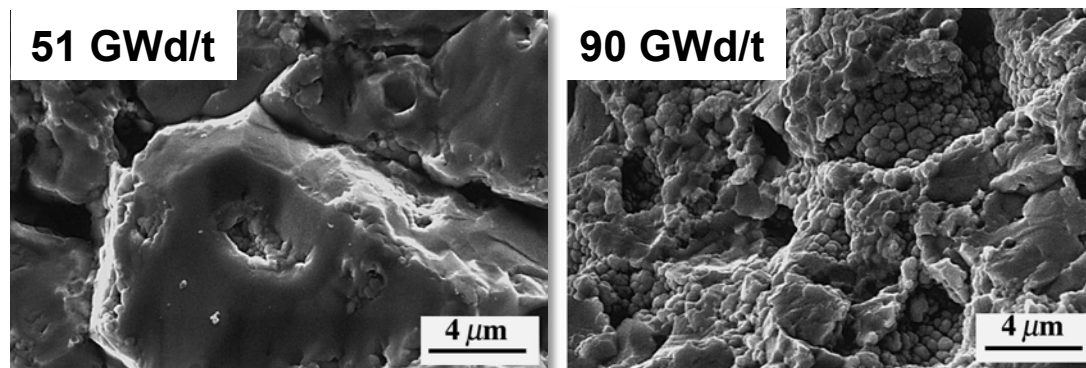
Summary

- The kMC-C.A. hybrid model reliably mimics static recrystallization behavior in a 2D models
- 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 Rios et al.

Questions

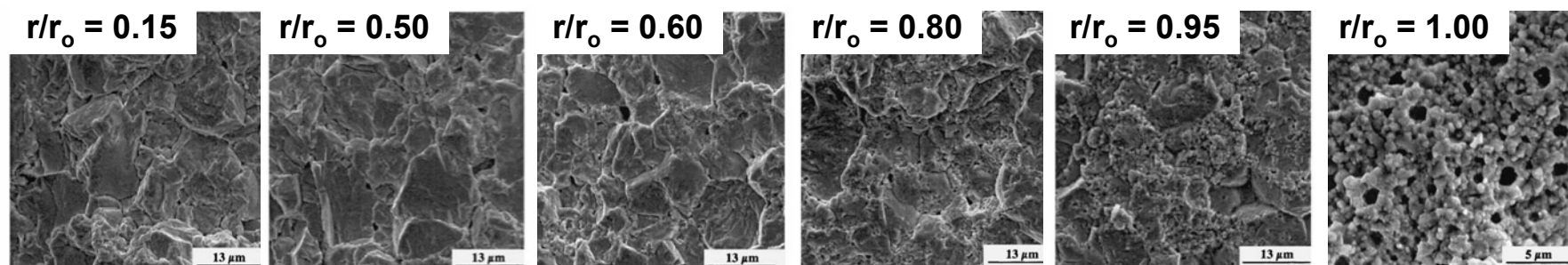
High Burn-Up Structure I

- 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



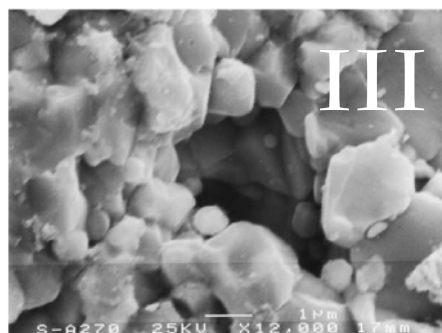
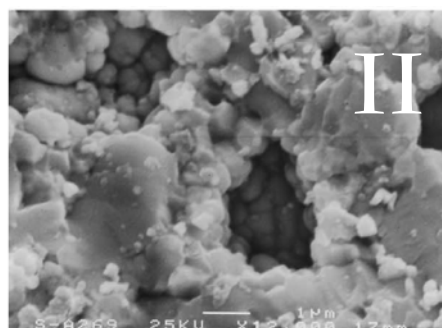
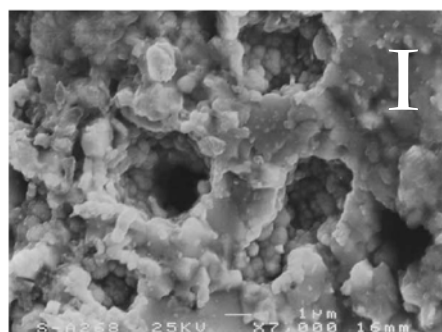
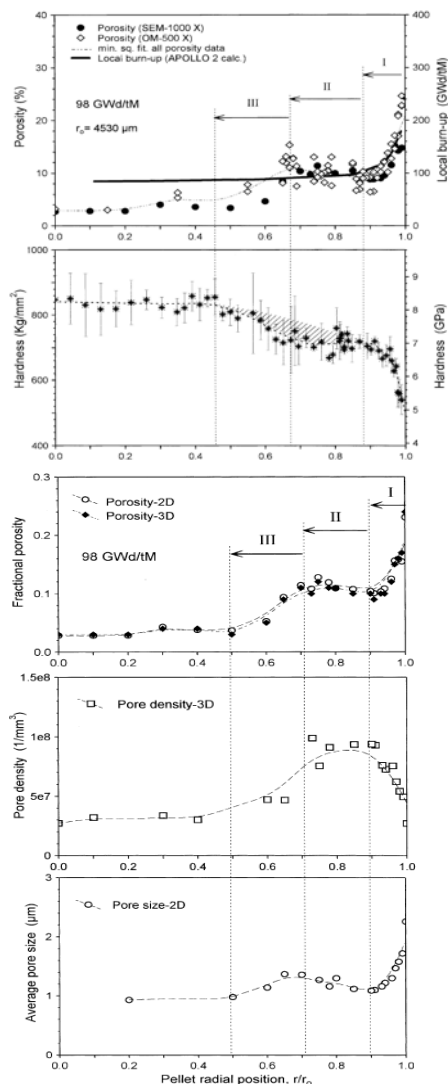
Une, et. al, JNM vol. 288, 2001

- 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.