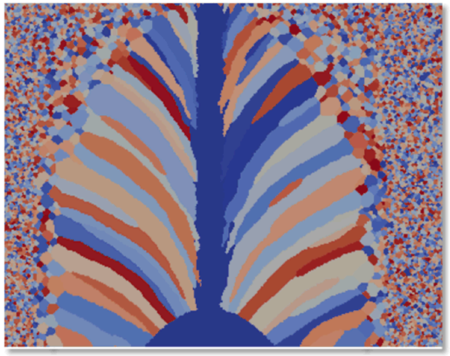
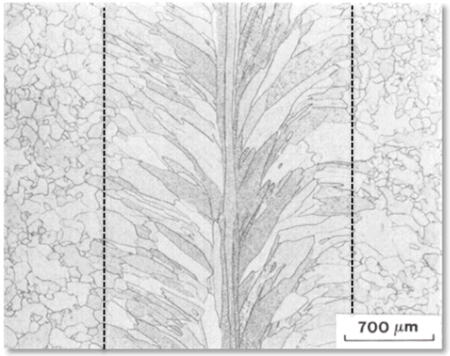
SAND2015-4249C

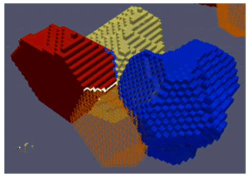
Meso-Scale Predictions of Microstructure Following Laser-Interaction via kMC Simulation

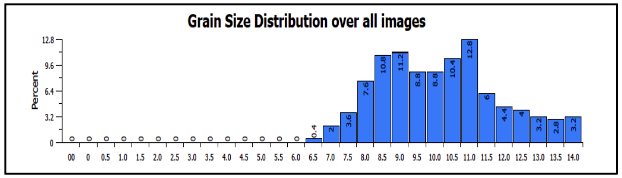
Exceptional service in the national interest

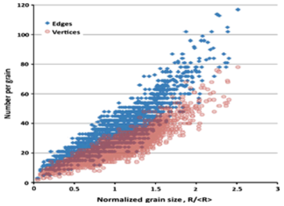
Sandia National Laboratories

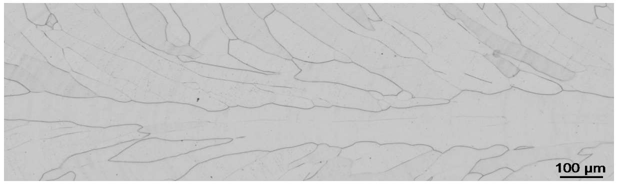












J. Madison, V. Tikare

[1]Sandia National Laboratories, Albuquerque NM

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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. 2015-XXXX

Outline

- Background
- Simulation Framework
- Equations of State
- Kinetics of Evolution
- Applicability to Welds
- Results
  - Experimental Results
  - Simulation Results
  - Experimental/Simulation Validation
- Future Work
- Summary

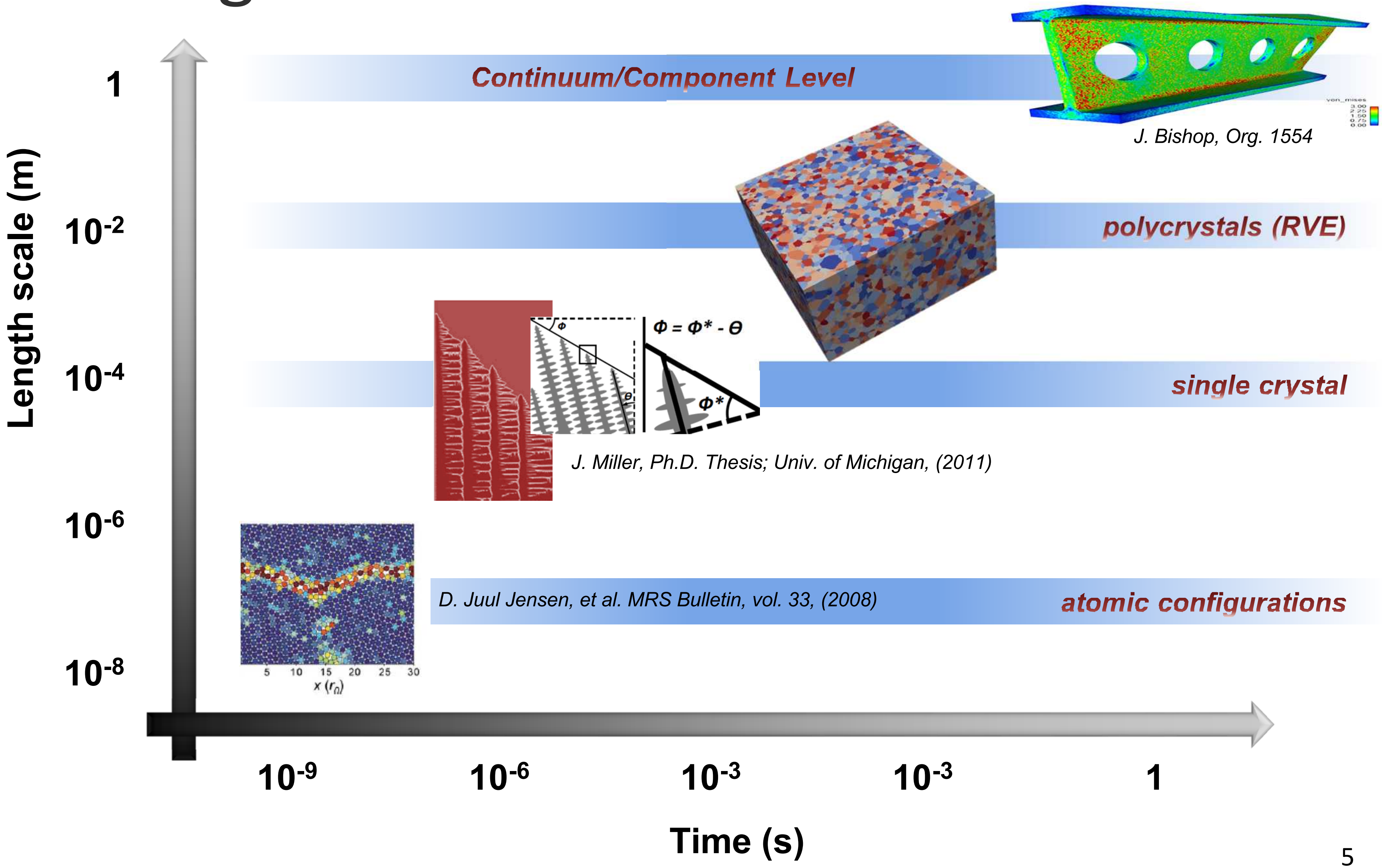
Background I

- **Metallurgists & ceramists have long agreed that most "homogenous" materials possess several levels of structure between the atomic and the macroscopic**
  - Dislocation networks
  - Precipitate dispersions
  - Grains & grain boundaries
  - Phases & phase boundaries
- **Microstructure influences, governs, dictates and/or explains**
  - Mechanical properties
  - Thermal properties
  - Electrical properties
  - Temporal behavior
- **Microstructural evolution has been a focus of study for over a century**
  - J.E. Burke & D. Turnbull, *Prog. Metal Phys.*, 3 (1952) p. 220

Background II

- **Computational simulations of microstructural evolution can be traced back to the 1950's**
  - R.L. Fullman, *Metal Interfaces* (Cleveland, OH: ASM, 1952), p. 179
  - manual calculations of grain growth
- **Many computational tools have been developed with a focus on microstructural evolution**
  - **Thermo-Calc –** thermodyanic predictions
  - **PanDat** – thermodynamic predictions
  - **ProCast –** solidification
  - **JMatPro –**
  - **Micress –**
  - **Dante –**
  - **LAMMPS –** molecular dynamic simulation
  - **VaSP –** density functional theory
  - **PrecipiCalc –**

Background III

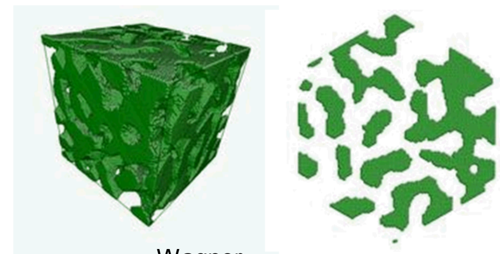


Simulation Framework

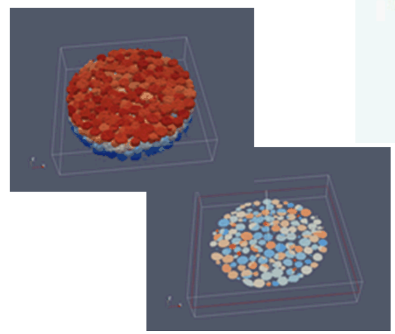
SPPARKS

Kinetic Monte Carlo via Stochastic Parallel PARticle Kinetic Simulator

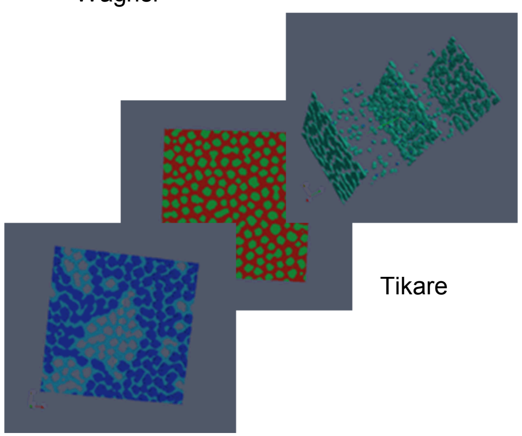
- Development a new user application for SNL's SPPARKS open-source environment
- Treat grain growth + dynamic recrystallization events simultaneously
- Incorporate probabilistic cellular-automaton approach to more accurately capture realistic kinetics (KJMA rates)
- Toward prediction of microstructural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



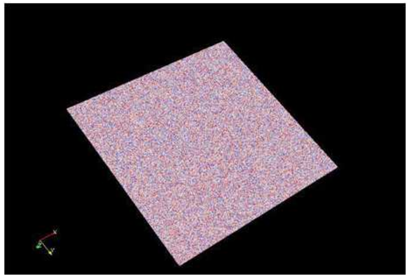
Wagner



Tikare & Garcia-Cardona



Tikare



http://spparks.sandia.gov

Thermodynamic Equations of State

- **Complex EOS can be constructed with two basic energy components :**
  - A volumetric free energy term, E_{vol}
  - An interfacial free energy term, E_{int}
  - These basic components are the basis for grain growth, recrystallization, sintering, abnormal grain growth, etc.

$$E = E_{vol} + E_{\text{int}}$$

$$E = \sum_{i=1}^{N} \left(E_{vol}(q_i) + \frac{1}{2} \sum_{j=1}^{n} J\left(1 - \delta_{ij}\right) \right)$$

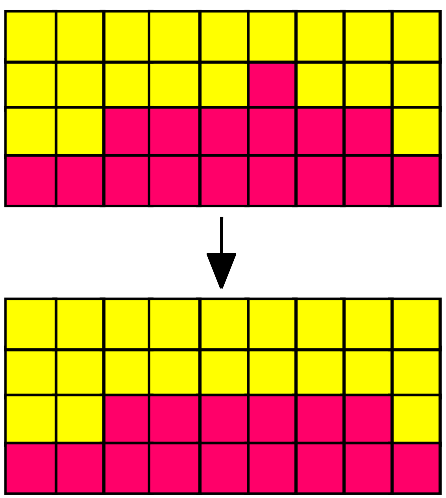
$$\begin{aligned} &where;\ N = \#\ of\ sites \\ &n = \#\ of\ neighbors \\ &j = neighboring\ sites \end{aligned}$$

Kinetics of Evolution I

- **Domain ensemble is statistically evolved to mimic atomistic diffusive processes.**
- **Boltzmann statistics are used to govern the evolutionary process**

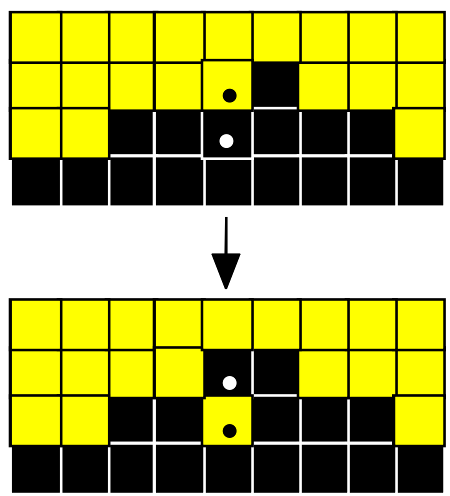
$$P = \begin{cases} 1 & for \quad E \leq 0 \\ \exp\left(\frac{-\Delta E}{kT}\right) & for \quad E > 0 \end{cases}$$

curvature driven grain growth



voxel membership change

diffusive particle migration



voxel membership change

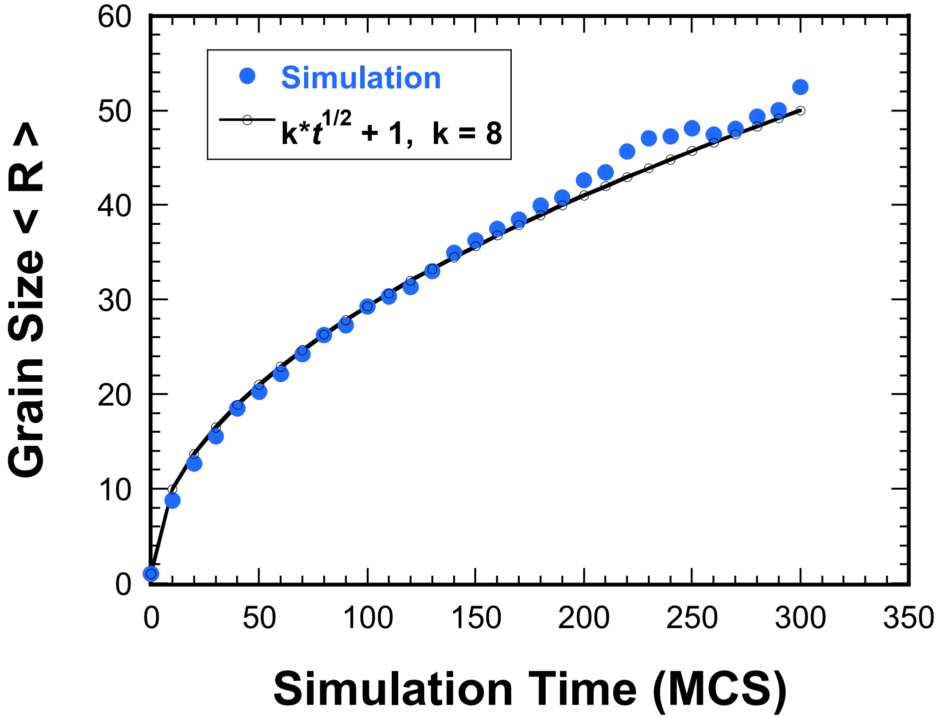
Ensemble evolution

Minimization of Total Free Energy

Kinetics of Microstructural Evolution

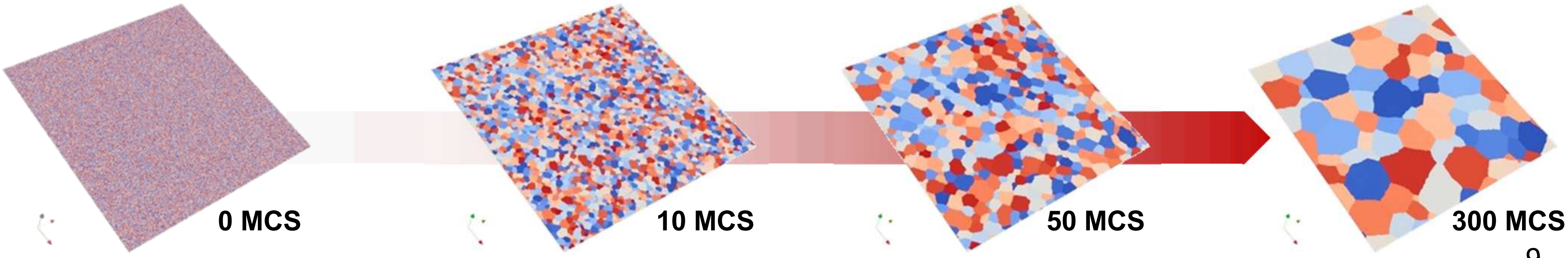
Kinetics of Evolution II

Traditional Grain Growth



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

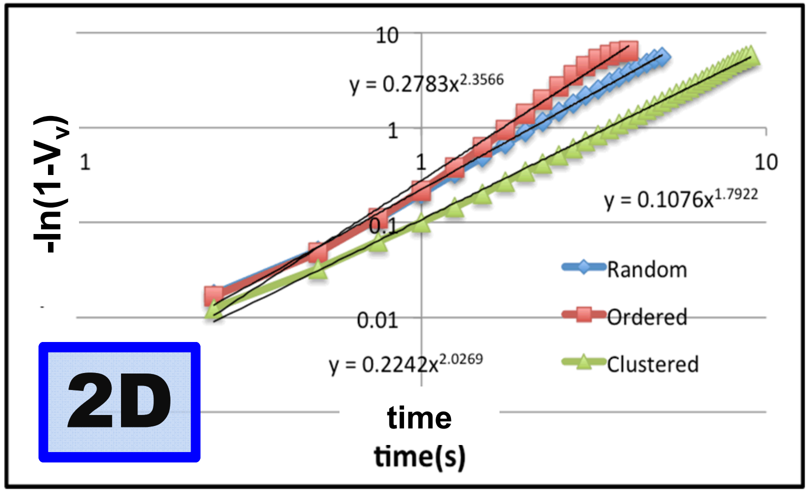
$$P = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T_S}\right) & if\ \Delta E > 0 \\ 1 & if\ \Delta E \leq 0 \end{cases}$$



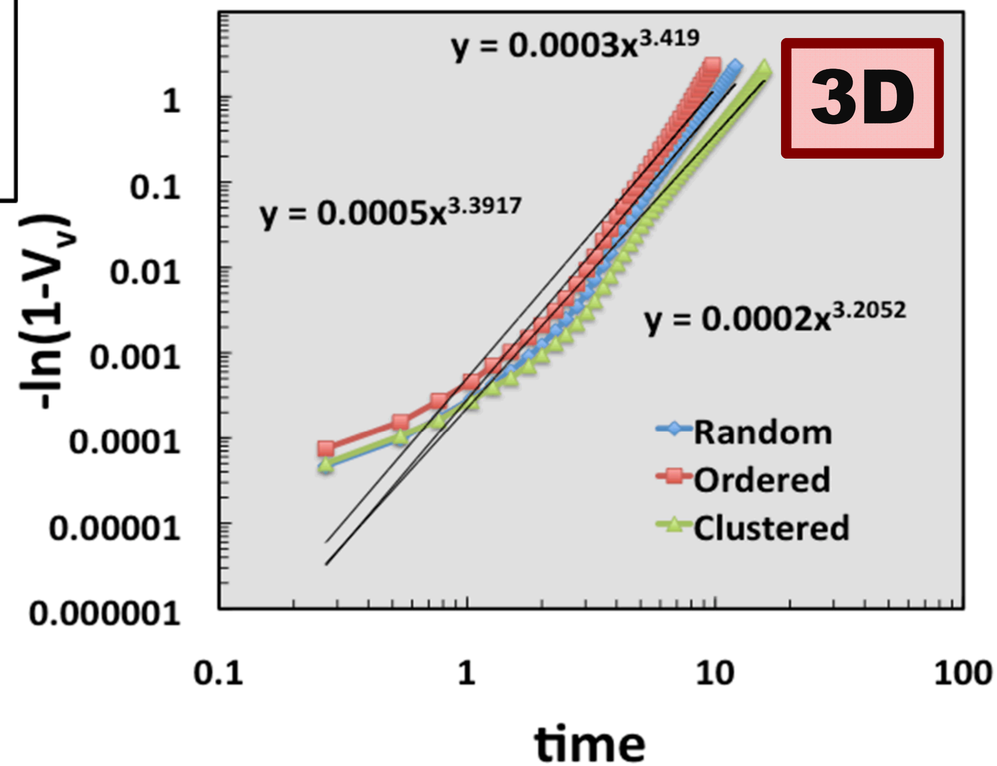
J. Madison, V. Tikare, L. Holm, ***J. Nuc. Mat***. vol. 425, (2012)

Kinetics of Evolution III

Recrystallization, KJMA Exponents

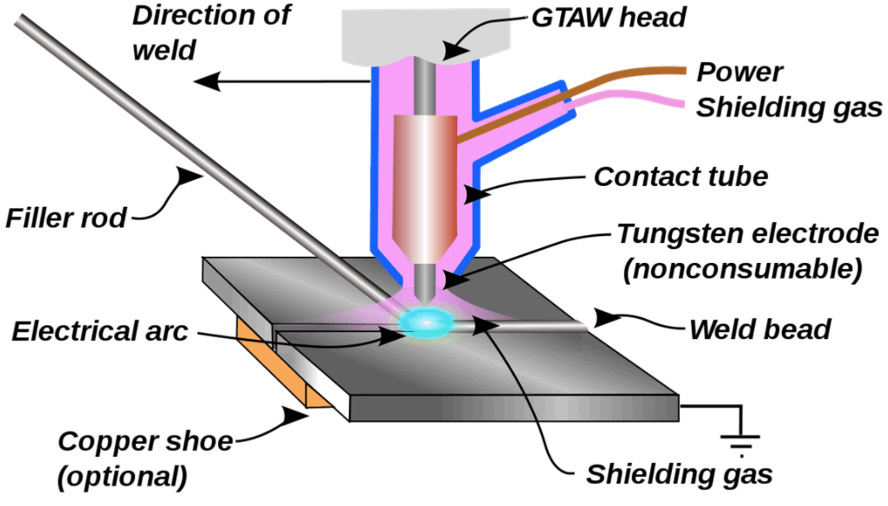


$$\log(-\ln(1-V_v)) = n\log(t)$$

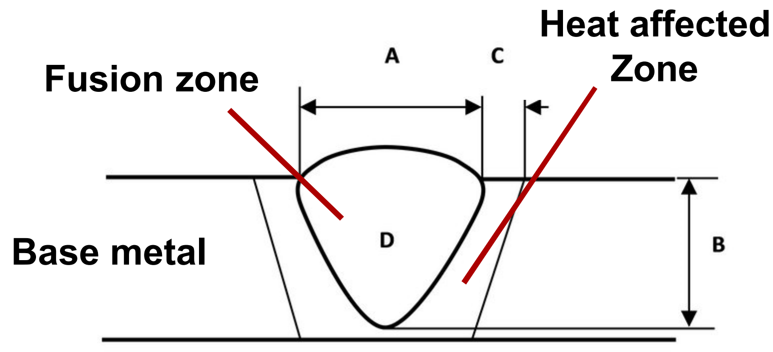


For site saturated nuclei
1D growth : $n \sim 1$
2D growth : $n \sim 2$
3D growth : $n \sim 3$

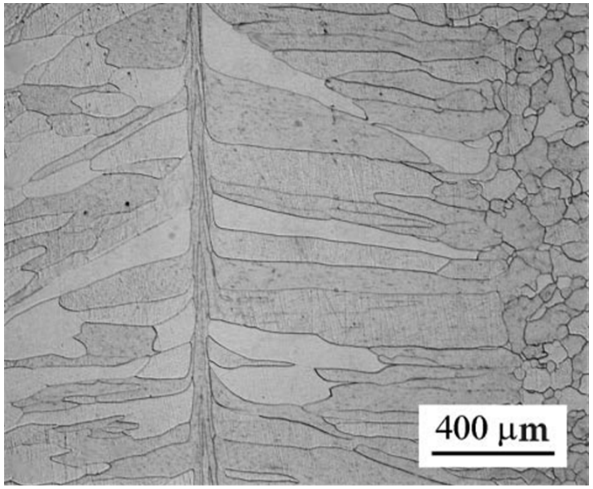
Applicability to Welds



Gas Tungsten Arc Welding



C. Neelamegam et al. *J. Int. Learning Sys. & Apps*, vol. 5 (2013), pp. 39-47



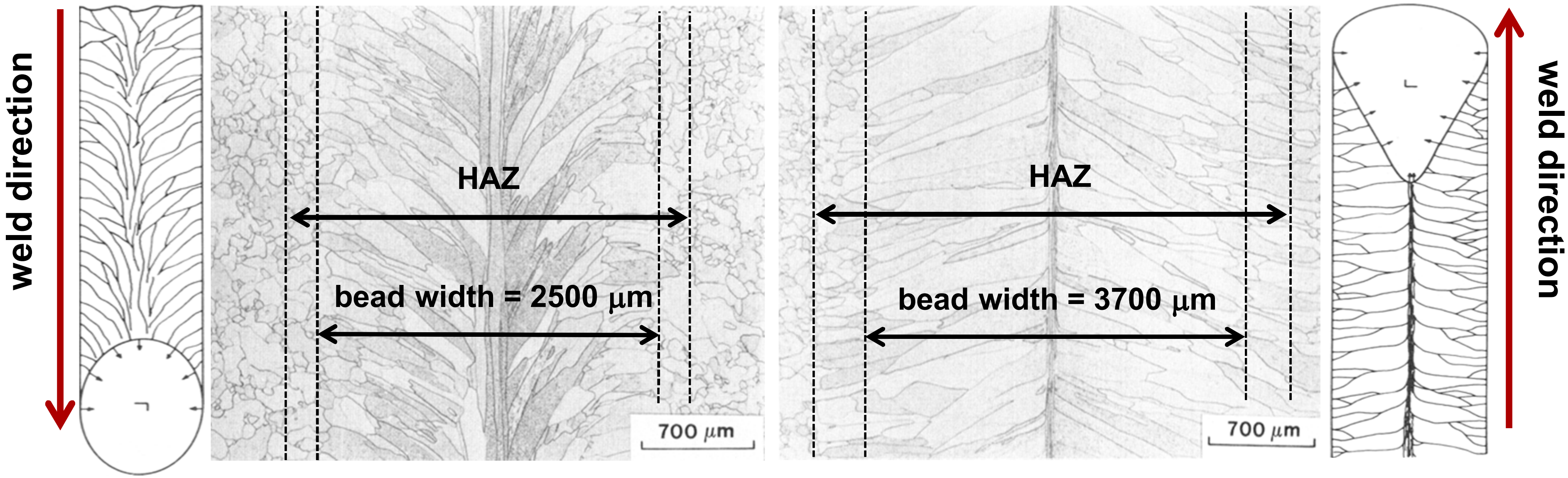
McKamey et al., *Sci &Tech. of Welding & Joining*, vol. 5 (2000), pp . 297-303

Experimental Microstructures

Welding of Iridium, DOP-26

Microstructure is primarily a function of :

- bead width: 3.7, 2.5 mm
- Heat input: determined bead width
- Weld speed: 76 cm/min



C. Liu & S. David, *Weld Metal Grain Structure and Mechanical Properties of a Th-Doped Ir-0.3 Pct W Alloy* **Met Trans A**. vol. 13 A, (1982) pp. 1043-1053

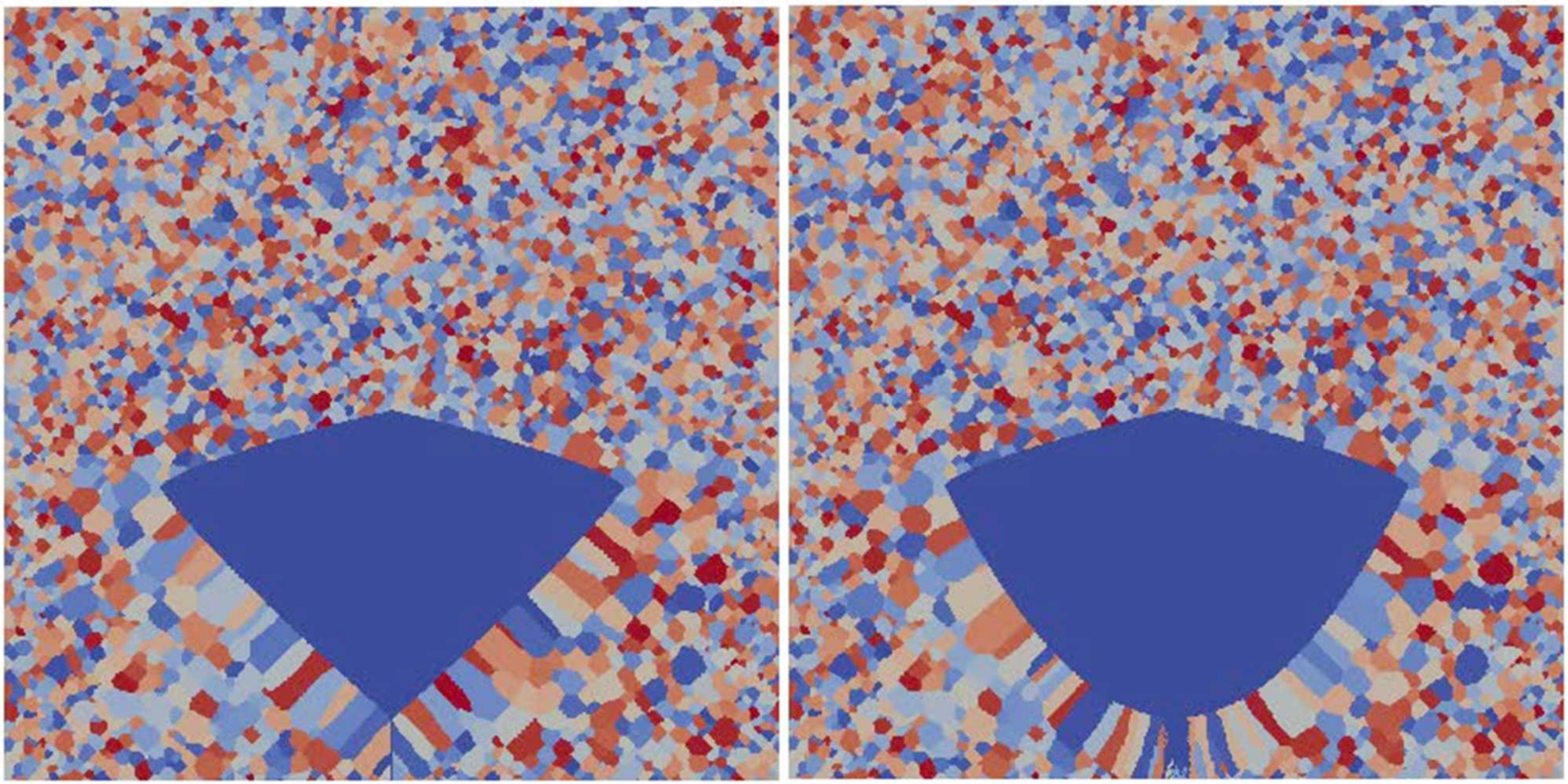
Simulated Microstructures

Base metal

HAZ

FZ

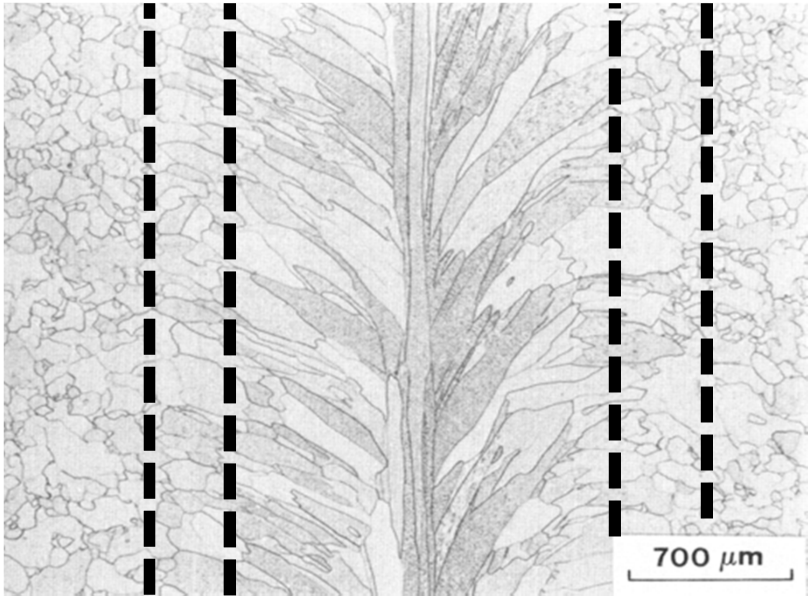
Grains grow epitaxially, perpendicular to iso-temperature lines



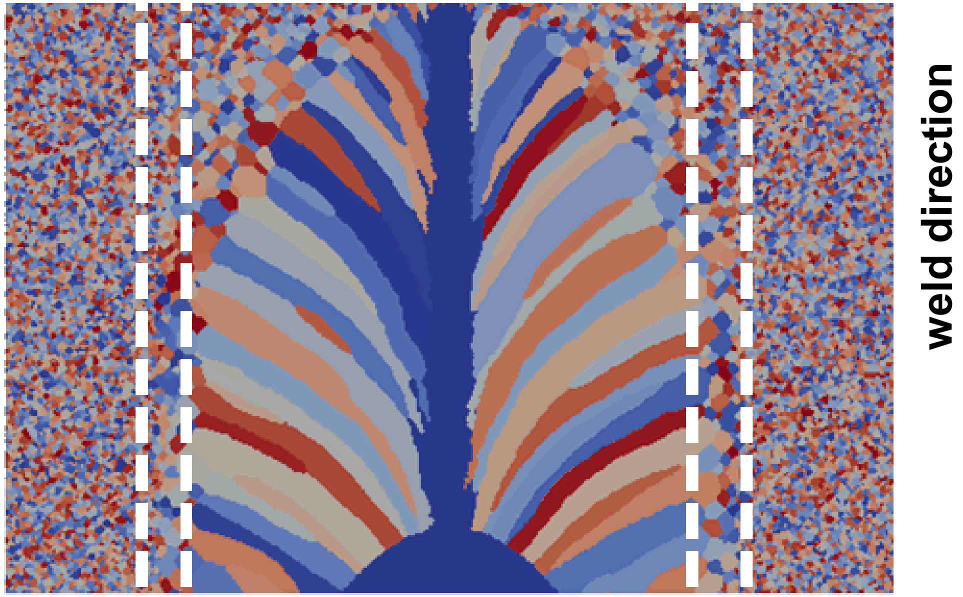
Experiment/Simulation Comparison

bead width = 2.5 mm
weld speed = 760 mm/min
weld grain size = 184 μm

spot size = 2.5 mm
heat source travel rate = 760 mm/min
weld grain size = 190 μm



C. Liu & S. David, ***Met Trans A***. vol. 13 A, (1982)



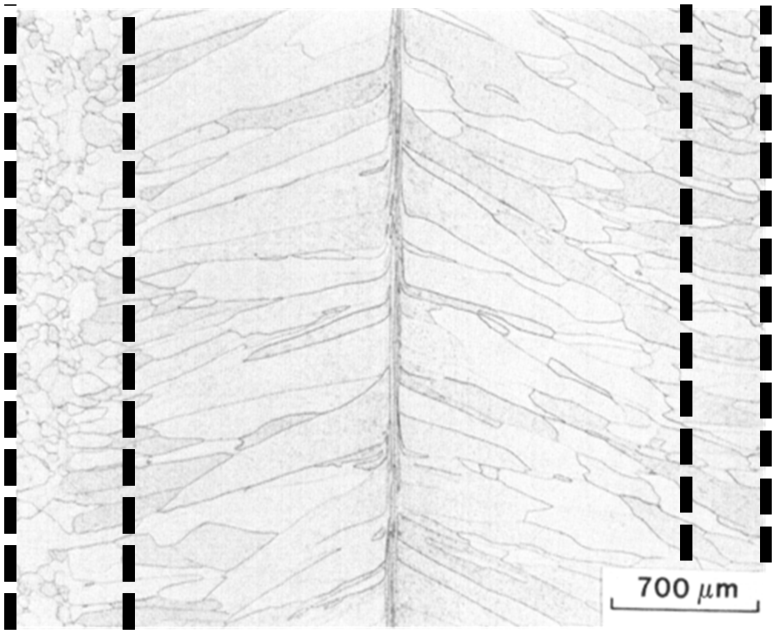
← Bead Width = 2500 μm →

← HAZ = 3125 μm →

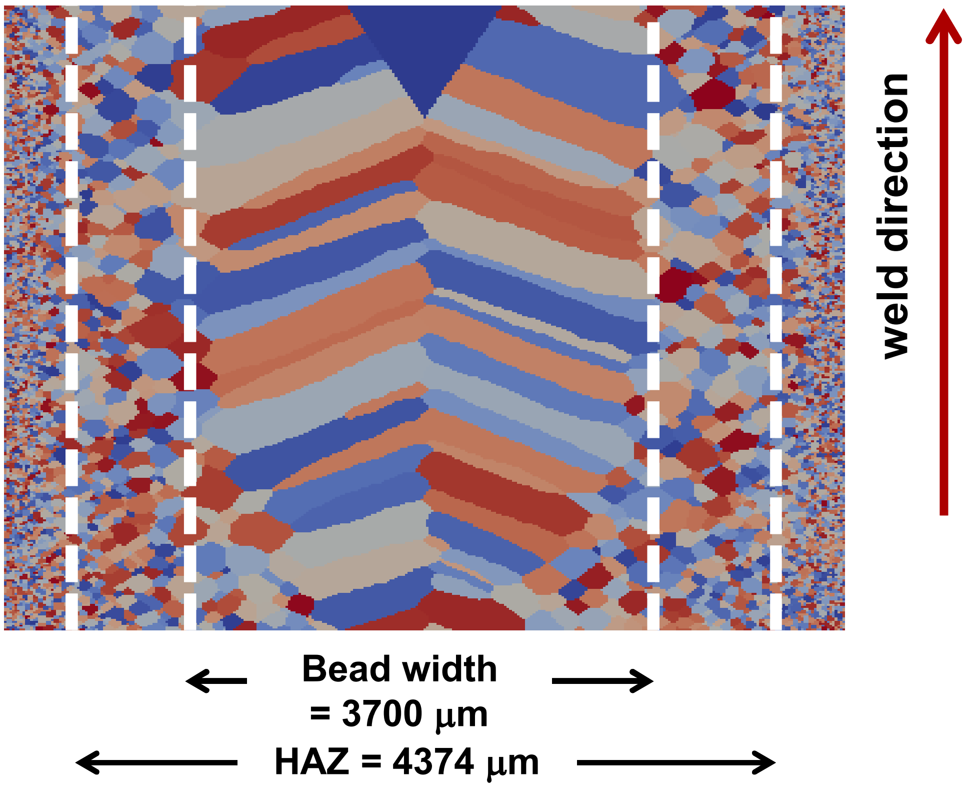
Experiment/Simulation Comparison

bead width = 3.7 mm
weld speed = 760 mm/min
weld grain size = 142 μm

spot size = 3.7 mm
heat source travel rate = 760 mm/min
weld grain size = 179 μm



C. Liu & S. David, ***Met Trans A***. vol. 13 A, (1982)



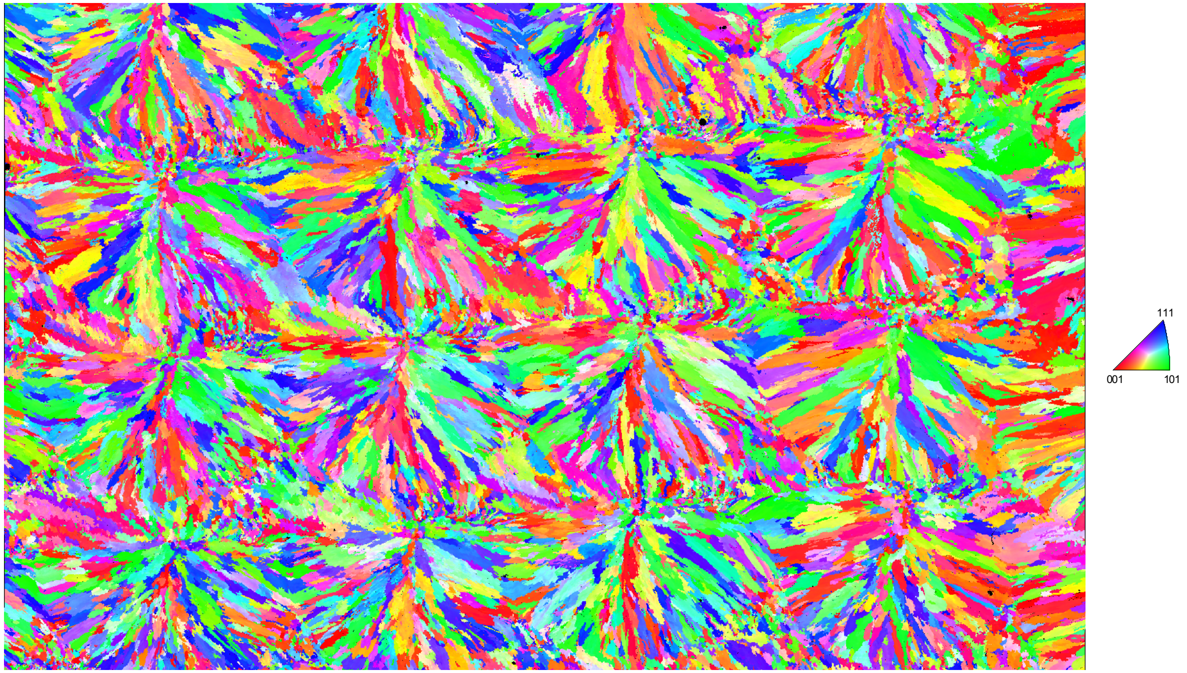
Summary

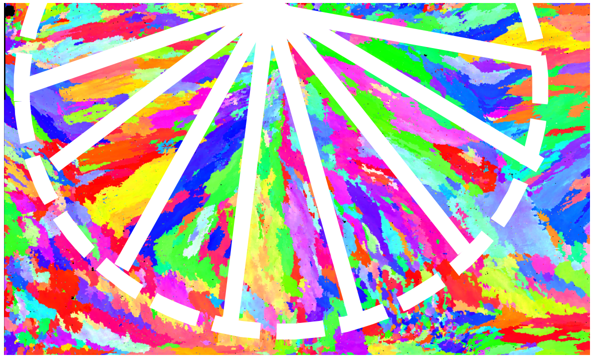
- **Developed and demonstrated a user-routine for SPPARKS which predicts experimental grain morphologies in the vicinity of a moving heat source**

- **SPPARKS simulation routine accepts the following as user inputs:**
  - Initial grain size
  - Welding spot size
  - Welding spot shape
  - Beam travel speed

- **SPPARKS simulation routine provides meso-scale grain predictions for welds in both 2 and 3-dimensions**

Application to Additive





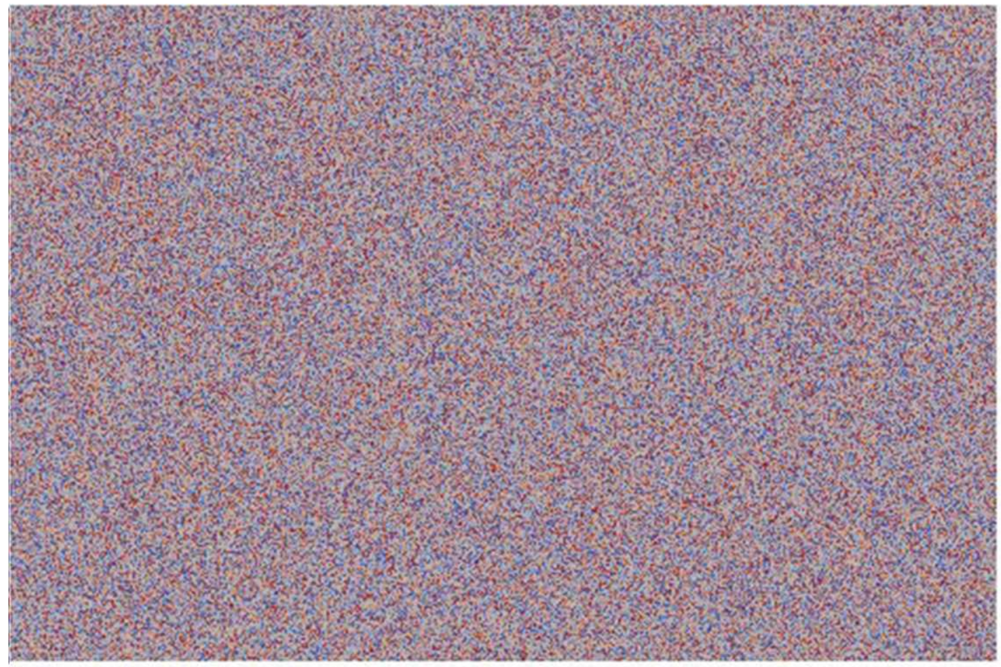
J. Michael (1800)
Montage EBSD Map
Laser Engineering Net Shape

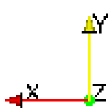
- *Crosshatched*
- *2 KW*

Simulate Solidification and Grain Growth with Correct Kinetics.

Initial grain size = 25 μm
X-dim = 4690 μm

Velocity = 76 cm/min





Bead width = 2500 μm

HAZ = 3125 μm

Algorithm Components

KINETIC MONTE CARLO

+

CELLULAR AUTOMATA

Stochastic, probability driven 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.

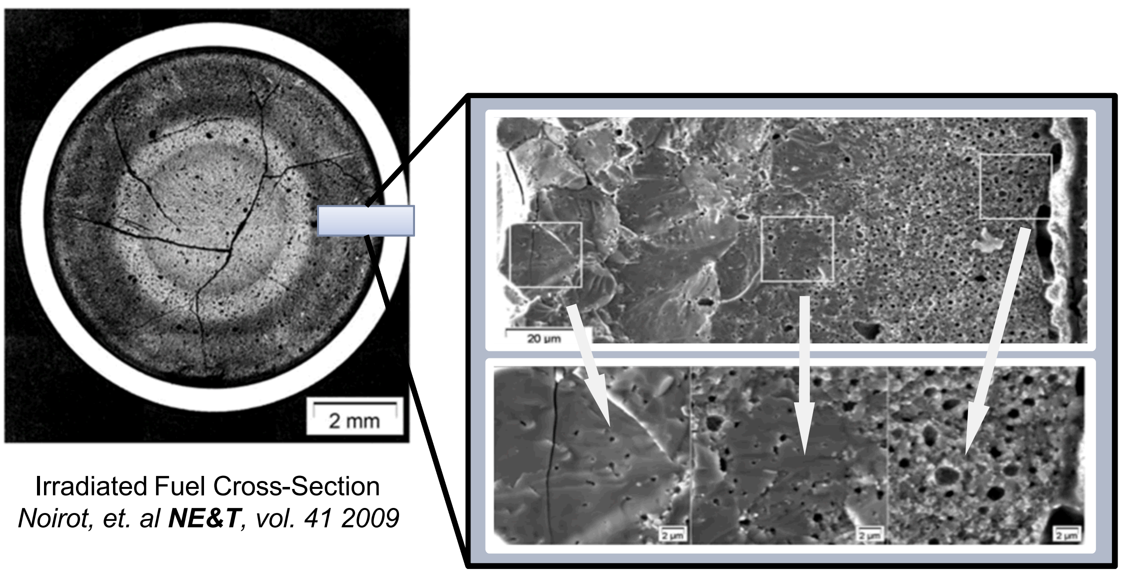
Deterministic, rule-based evolution

[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.

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

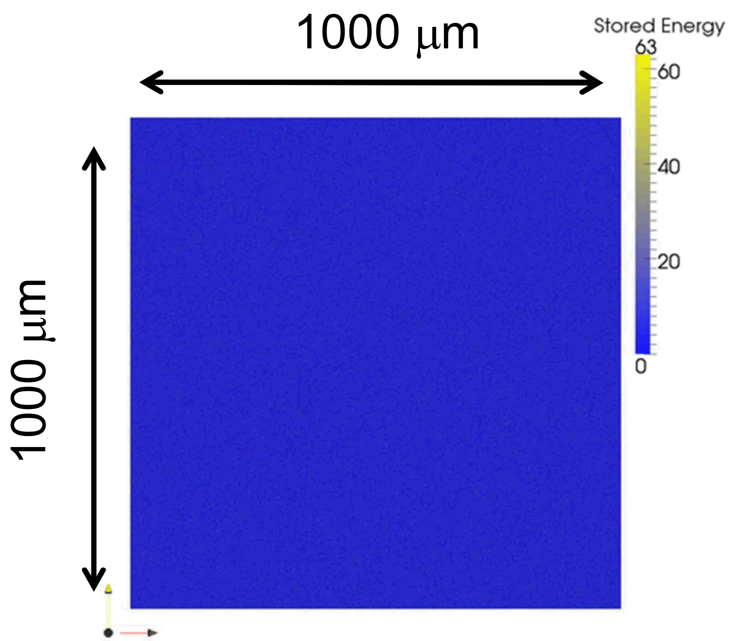
Tremendous Variation In Microstructure

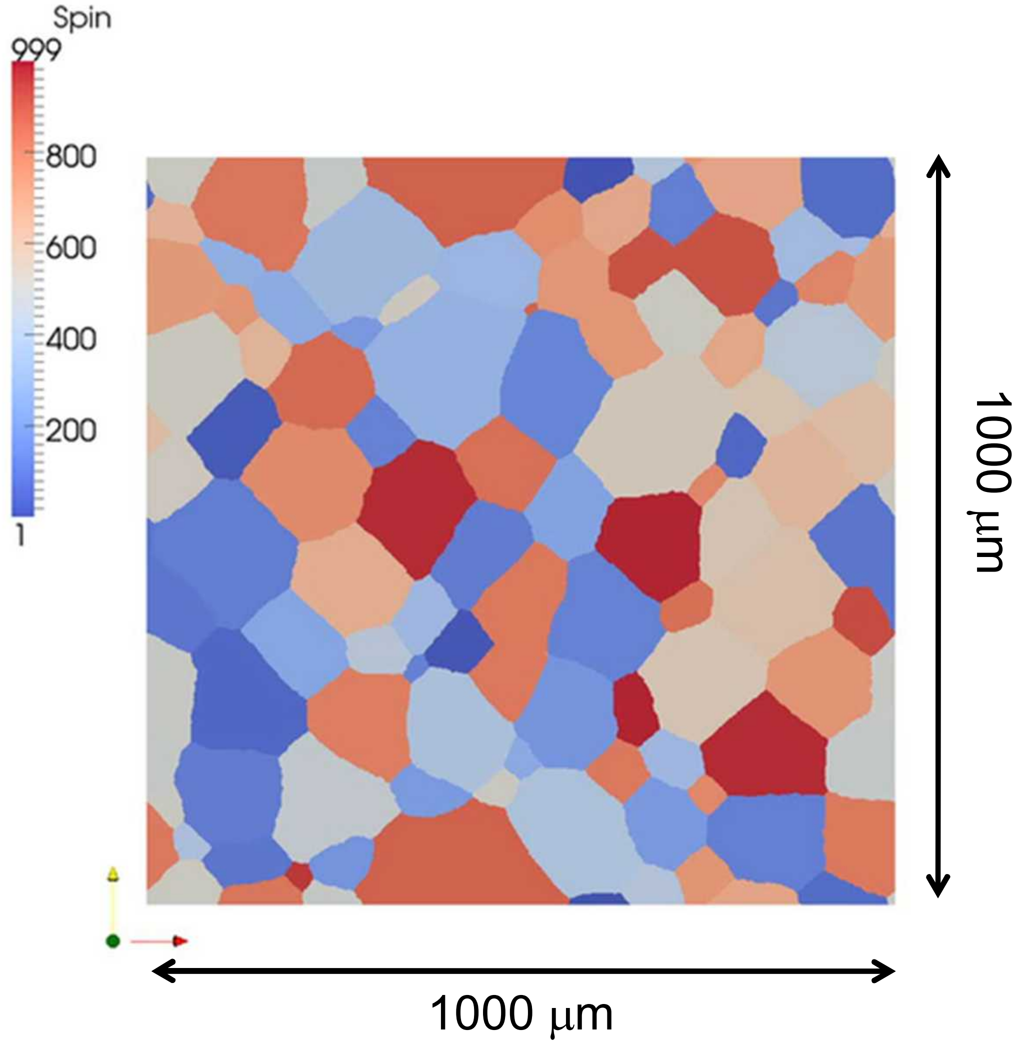
1. Grain size
2. Porosity
3. Percolation
3. Composition
4. Hardness

Sandia National Laboratories

Background III

$$\Omega(i,t+1) = \Omega(t) + \Delta t\,(r_i)$$



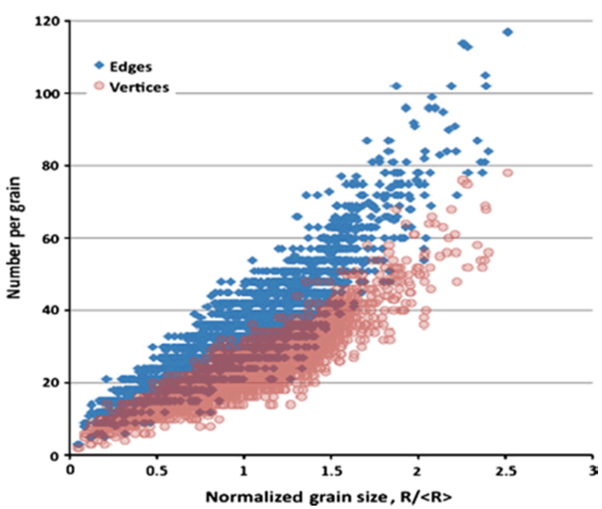


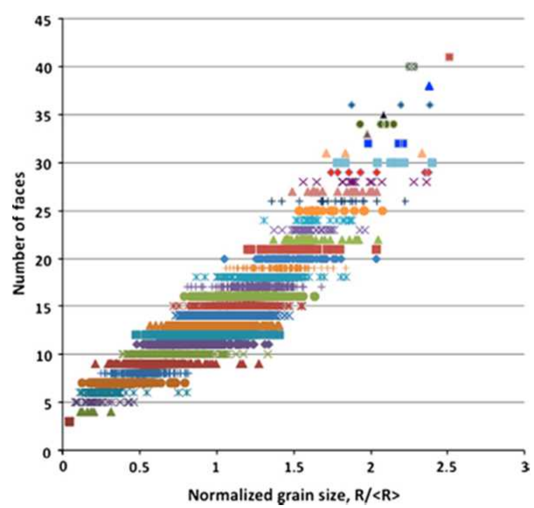
8 MCS / frame
1000 spins
1000 x 1000 x 1
Initial Grain Size <R> = 100
Average <R> During Recrystallization = 5

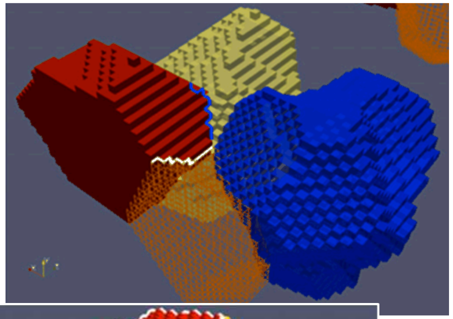
User Defined parameters: (*g*) threshold, (η) nucleation rate, (*M*) boundary mobility, (*r*) recrystallization rate

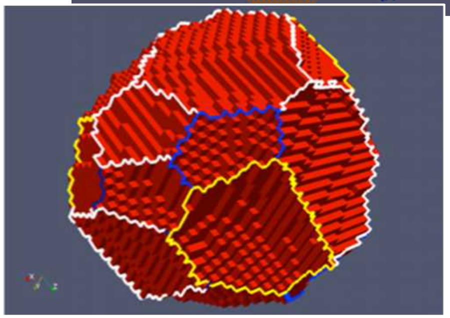
Background IV

- 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







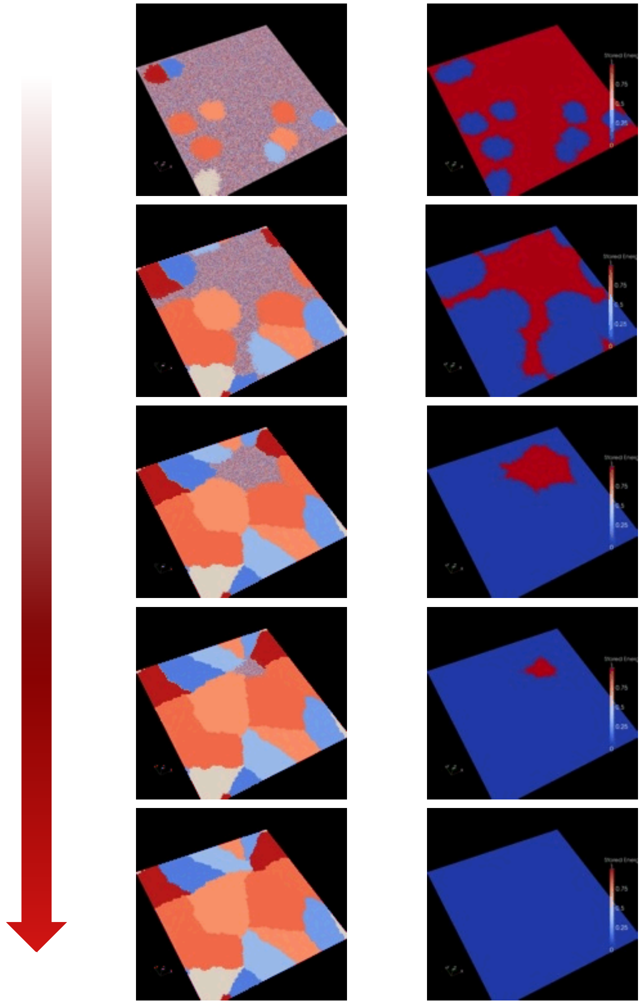


❖ Z. Sun, V. Tikare, B. R. Patterson and A. P. Sprague: *Comp. Mat. Sci.*, 2012, vol. 55 pp. 329-36.

C.A. for Recrystallization

Sandia National Laboratories

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



spins stored energy

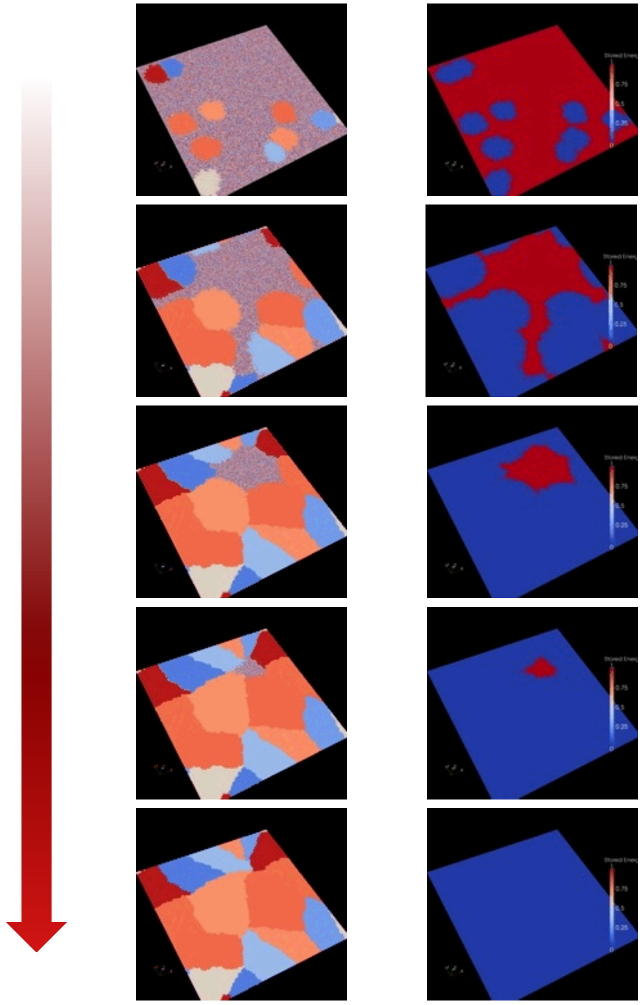
$$if\ \Omega_i < \Omega_j^{initial} \begin{cases} \Omega_j = \Omega_i \\ spin_j = spin_i \end{cases}$$

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

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

C.A. for Recrystallization

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



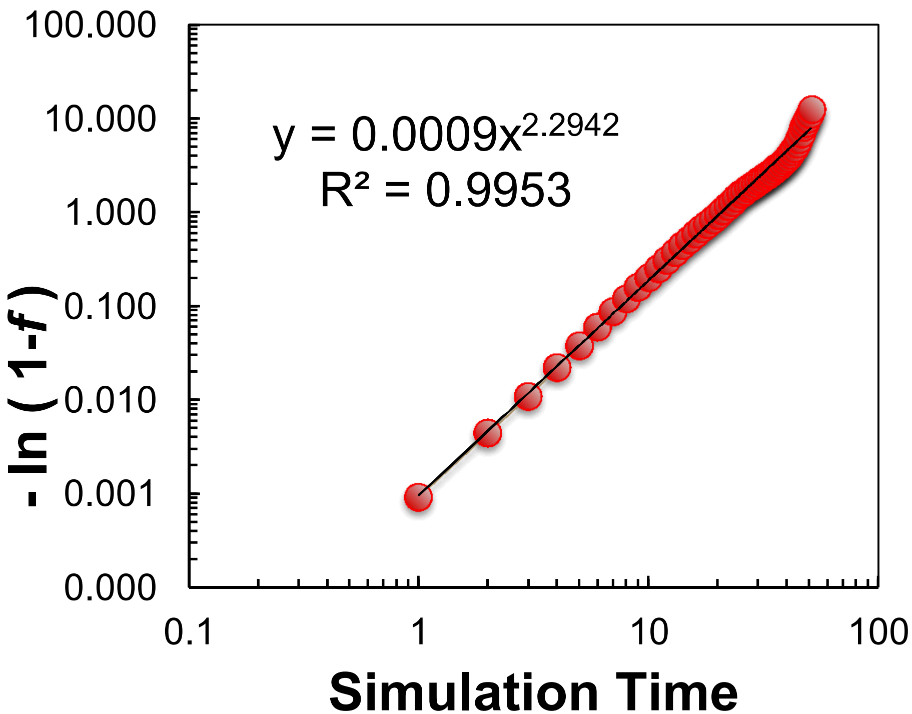
spins stored energy

$$Spins = 100$$

$$Total\ Sites = 250\,000$$

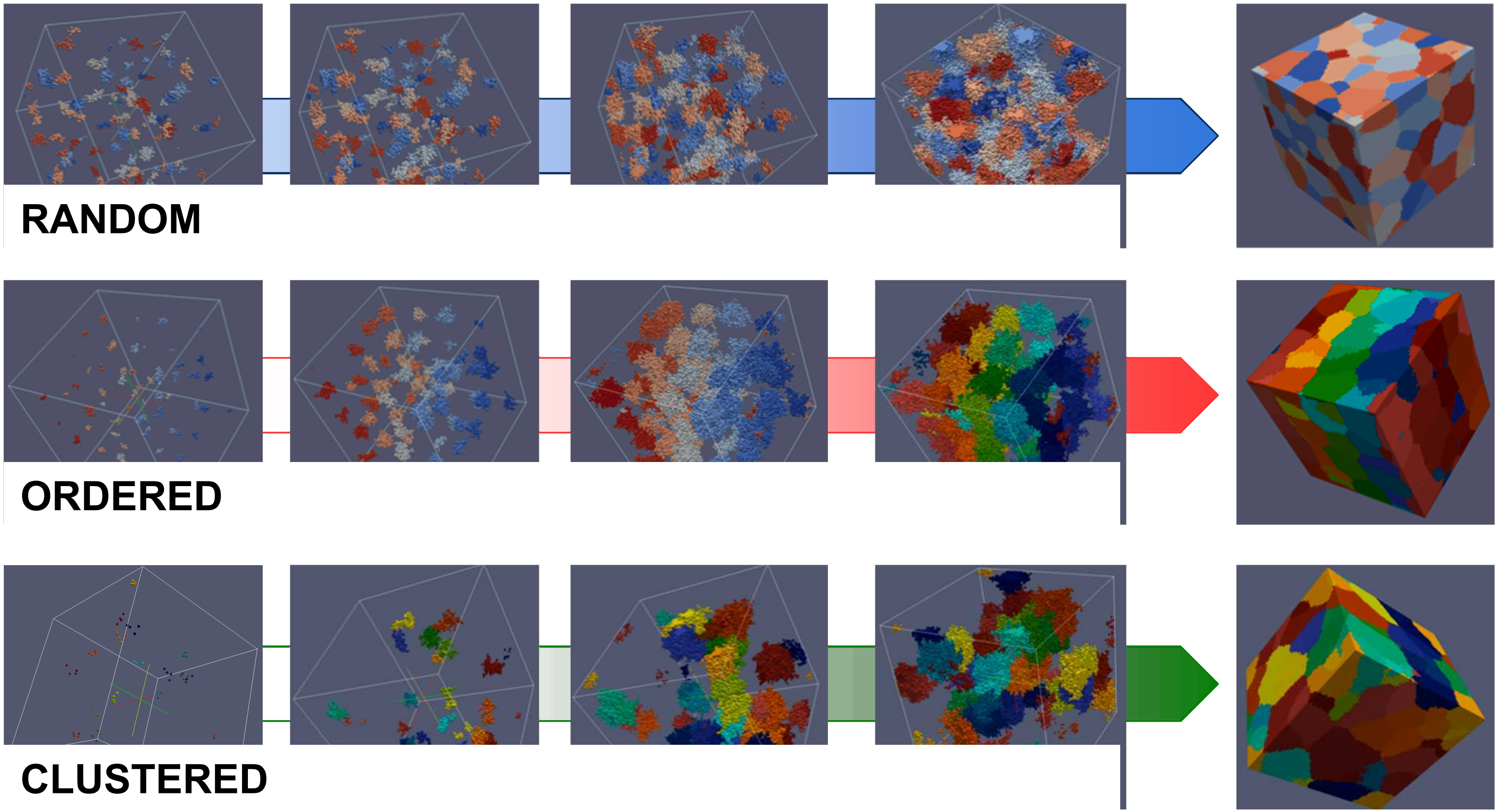
$$Total\ N_{accepted} = 247\,418$$

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

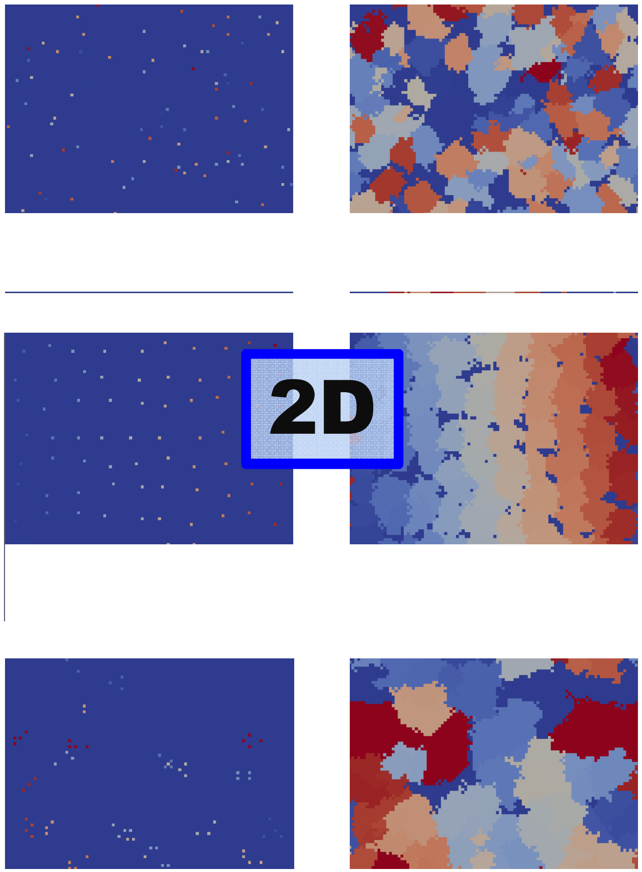


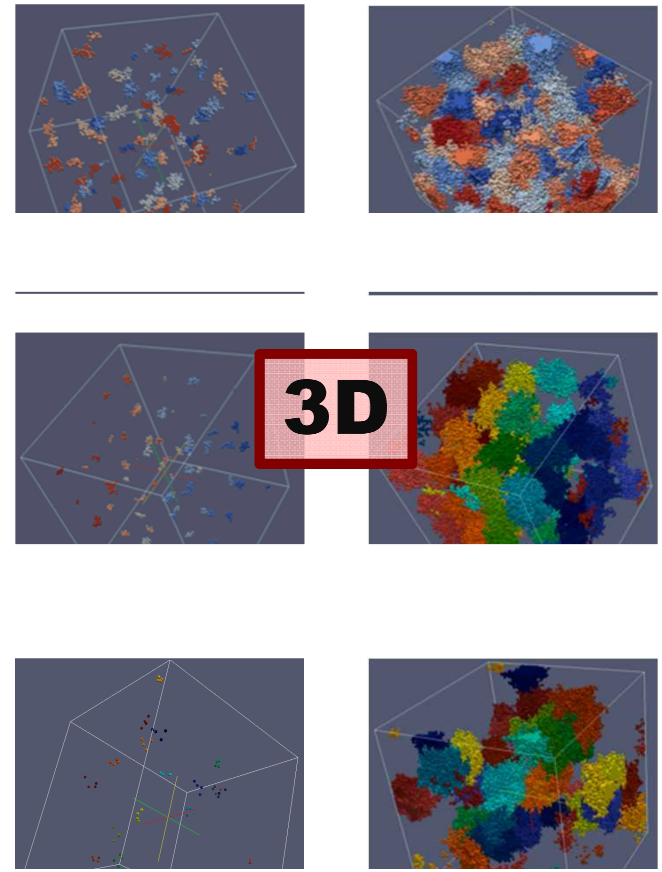
Nuclei Instantiation

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



2D & 3D Domains





RANDOM

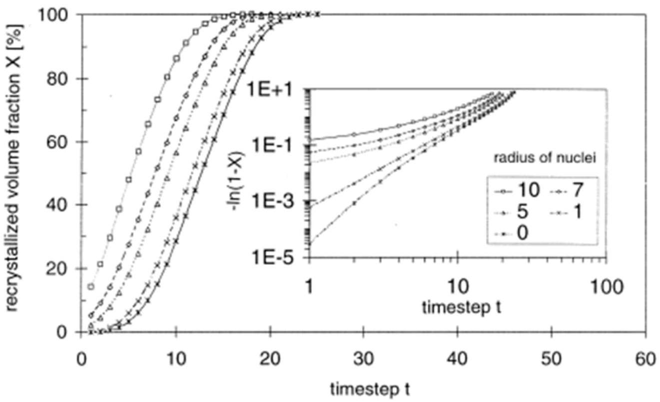
ORDERED

CLUSTERED

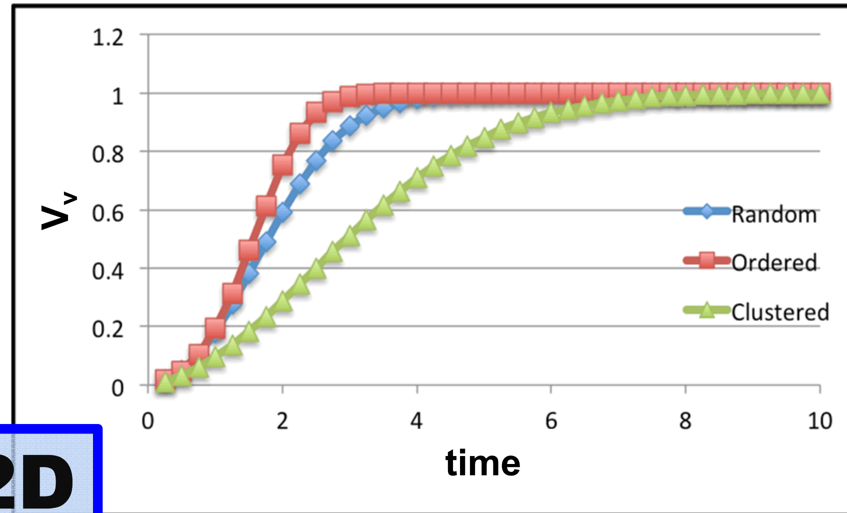
500 x 500 x 1
Instantiated Nuclei = 1000 = 0.4%
Site saturated Static ReX

100 x 100 x 100
Instantiated Nuclei = 1000 = 0.1%
Site Saturated Static ReX

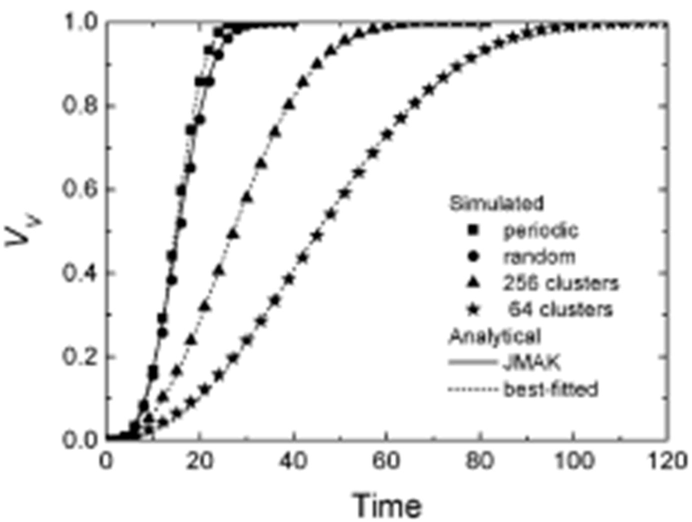
Volume Fraction



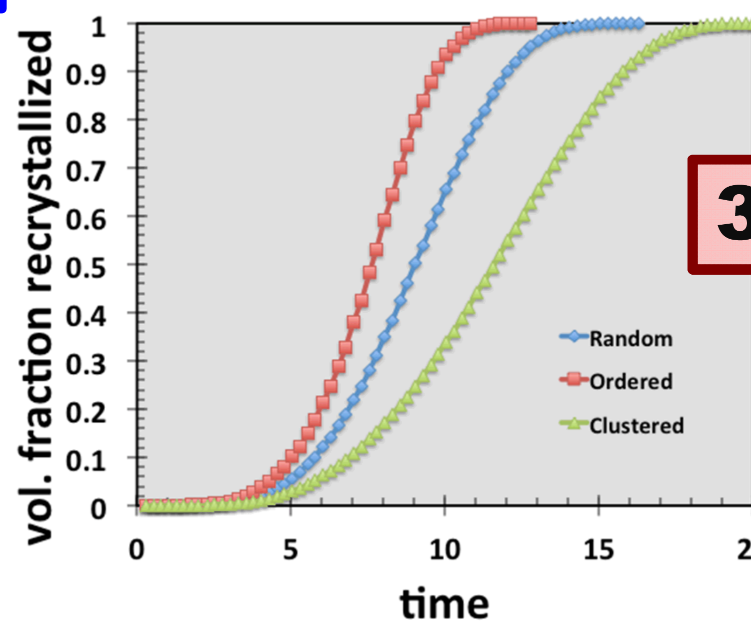
Marx et al: *Acta Mat.*, 1999, vol. 47 pp. 1219-1230.



2D

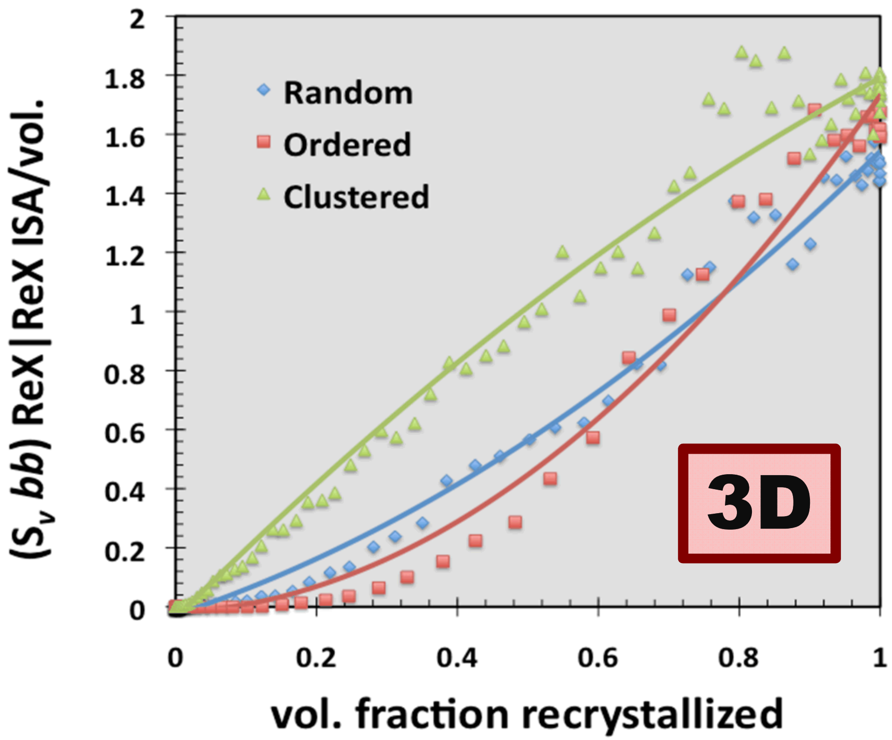


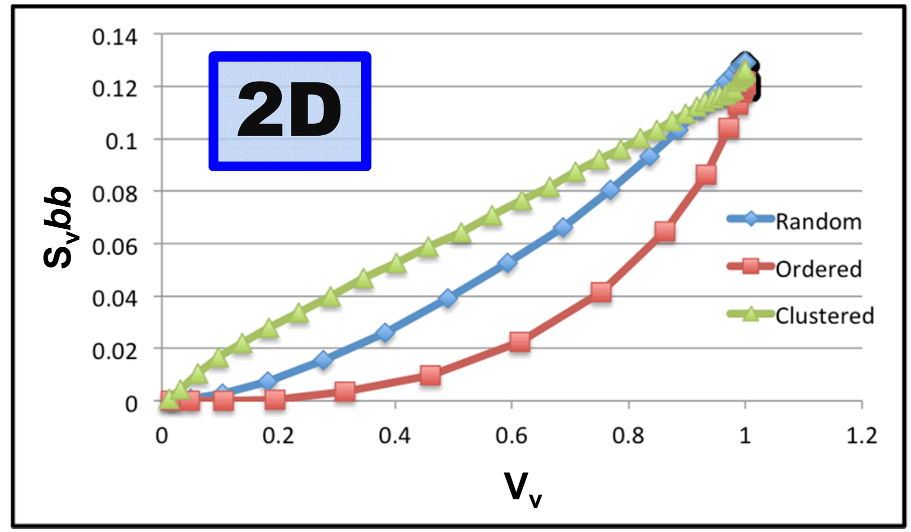
P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro: *Acta Mat.*, 2007, vol. 55 pp. 4339-48.

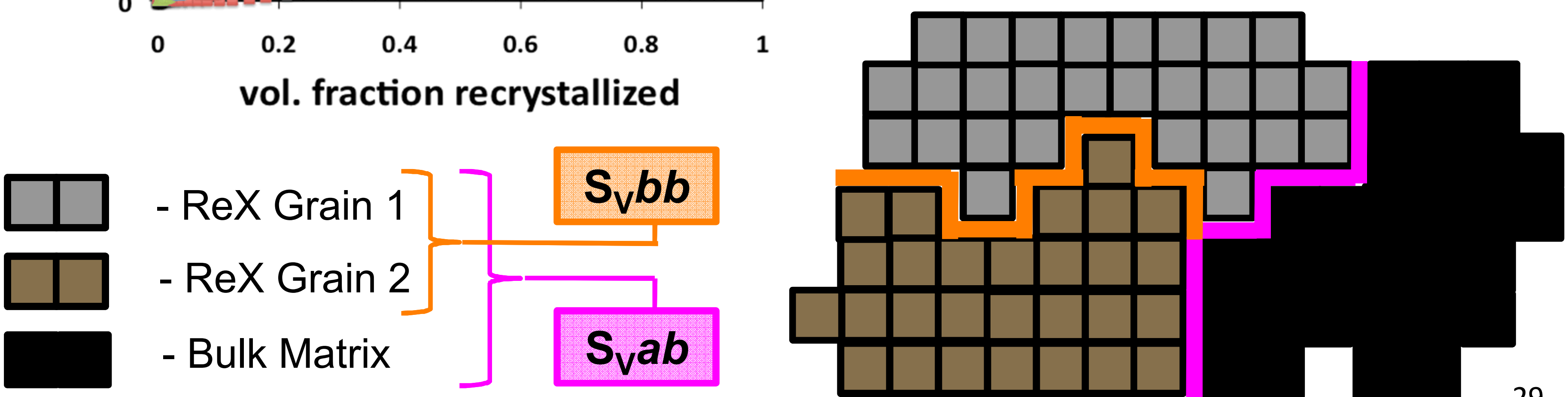


3D

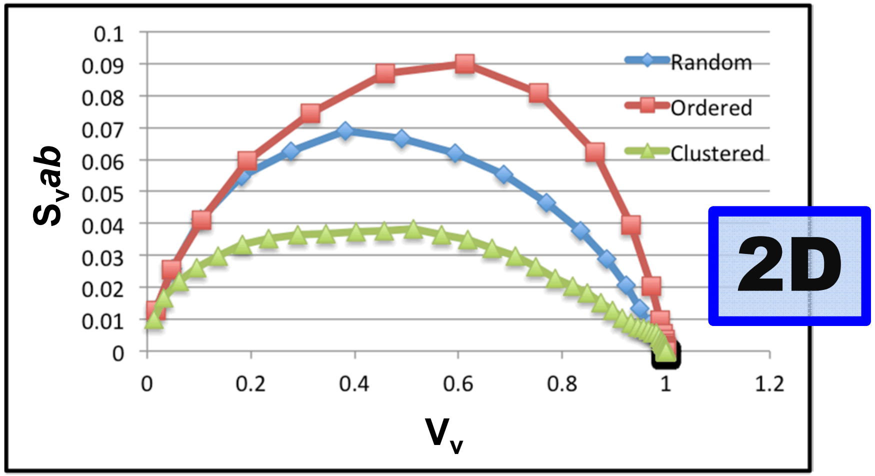
Interfacial Surface Area I

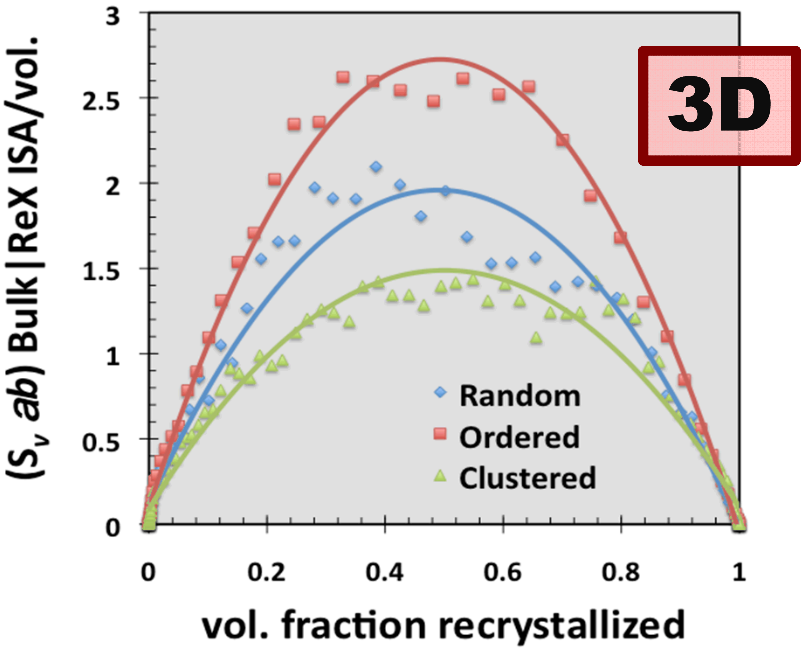


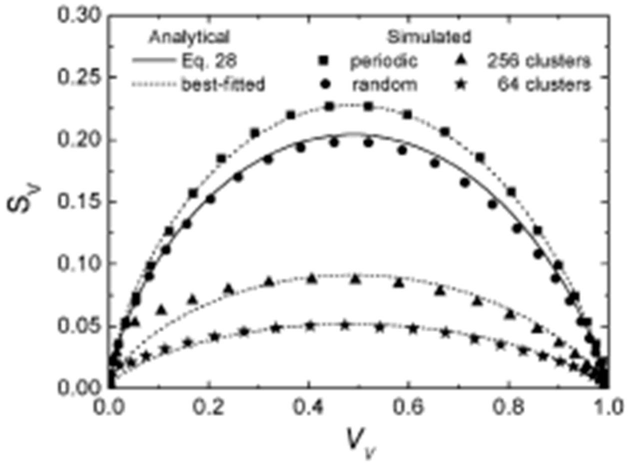




Interfacial Surface Area II



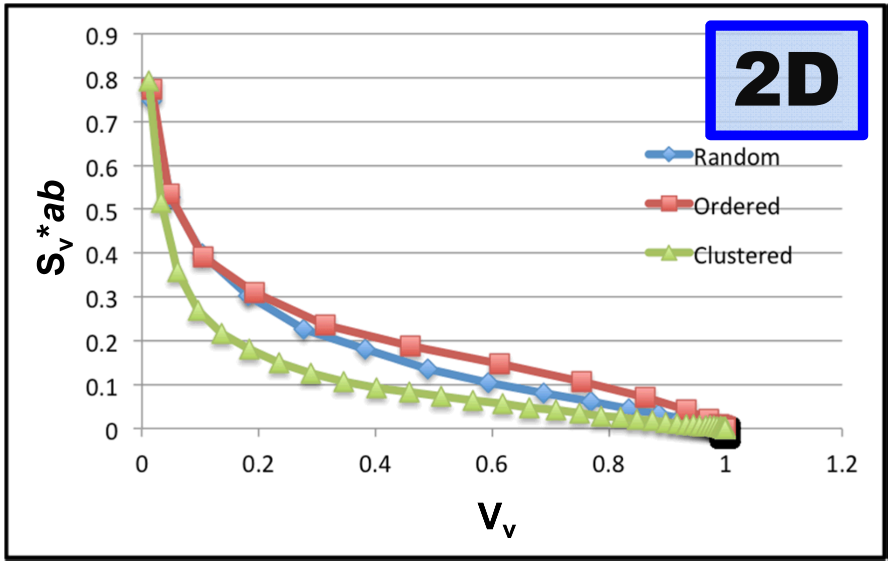


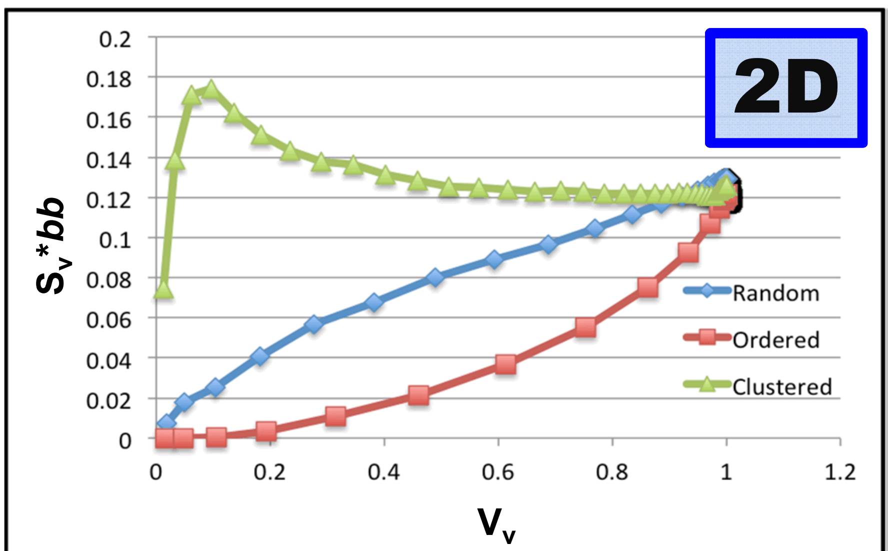


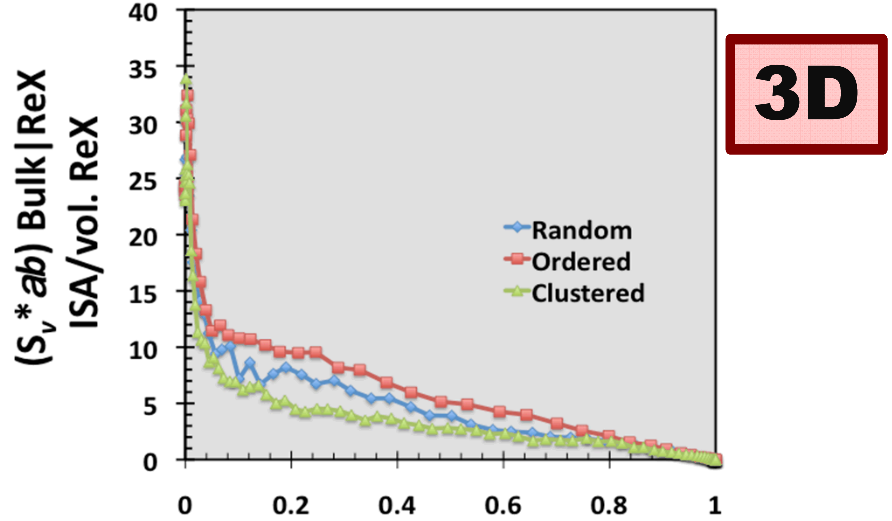
P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro: *Acta Mat.*, 2007, vol. 55 pp. 4339-48.

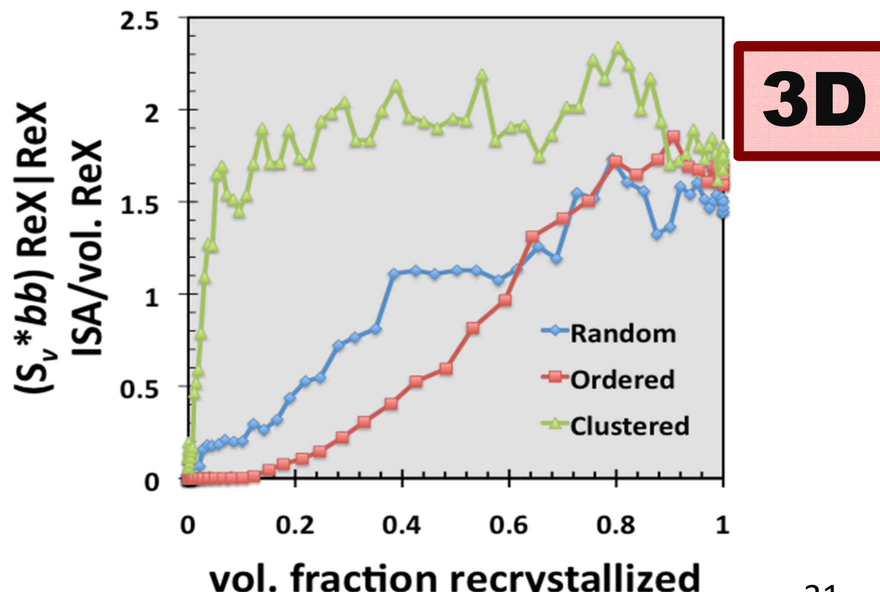
Sandia National Laboratories

Interfacial Surface Area III

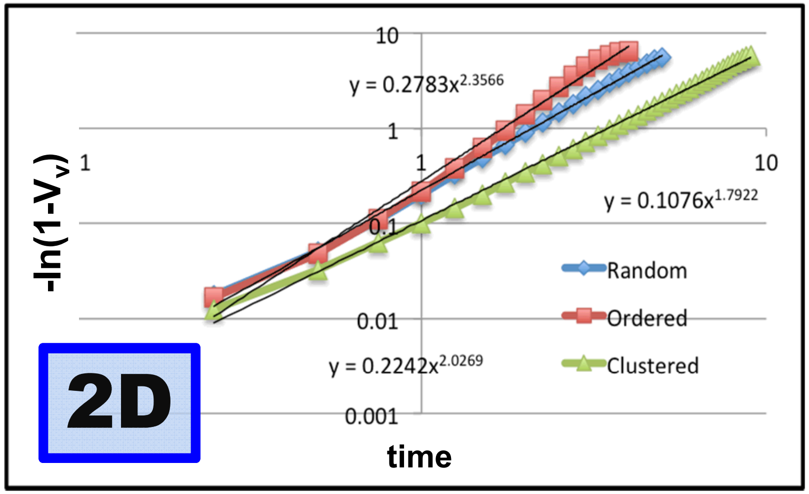






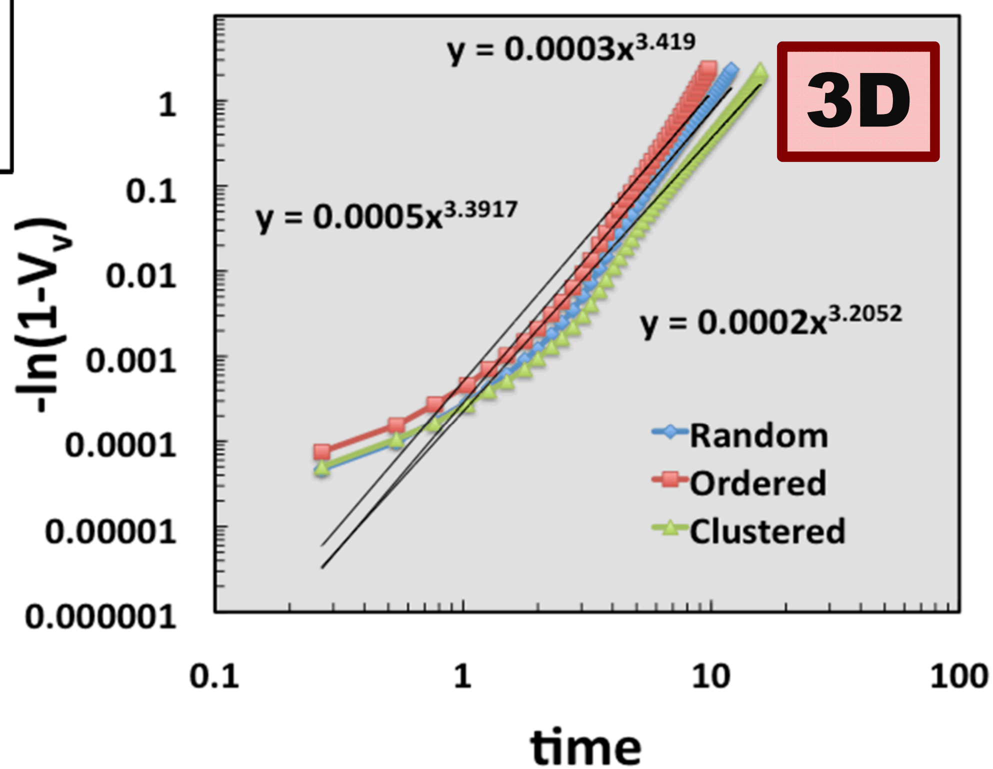


KJMA Exponent



$$\log(-\ln(1-V_v)) = n\log(t)$$

For site saturated nuclei
1D growth : $n \sim 1$
2D growth : $n \sim 2$
3D growth : $n \sim 3$

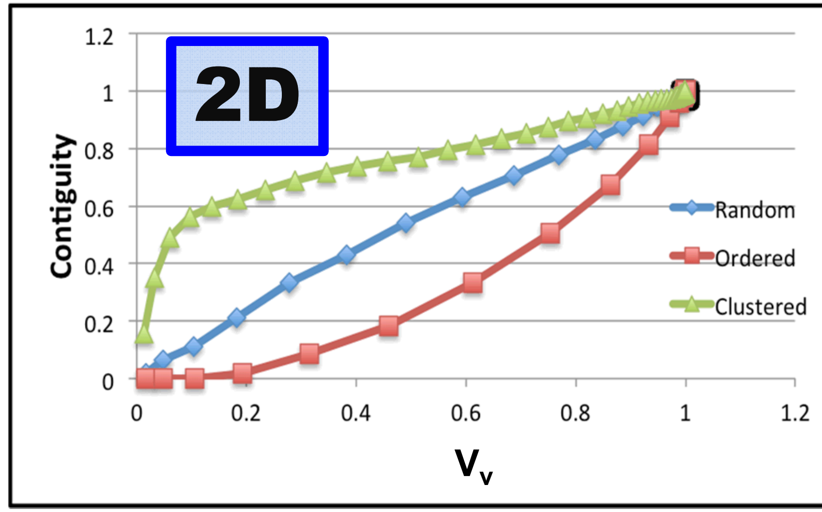


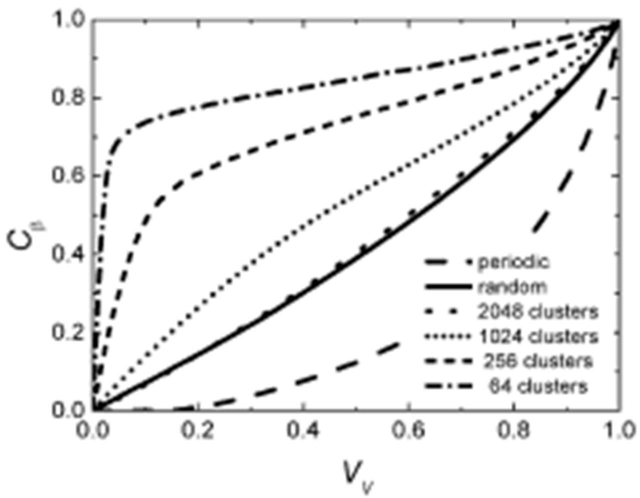
Contiguity

Sandia National Laboratories

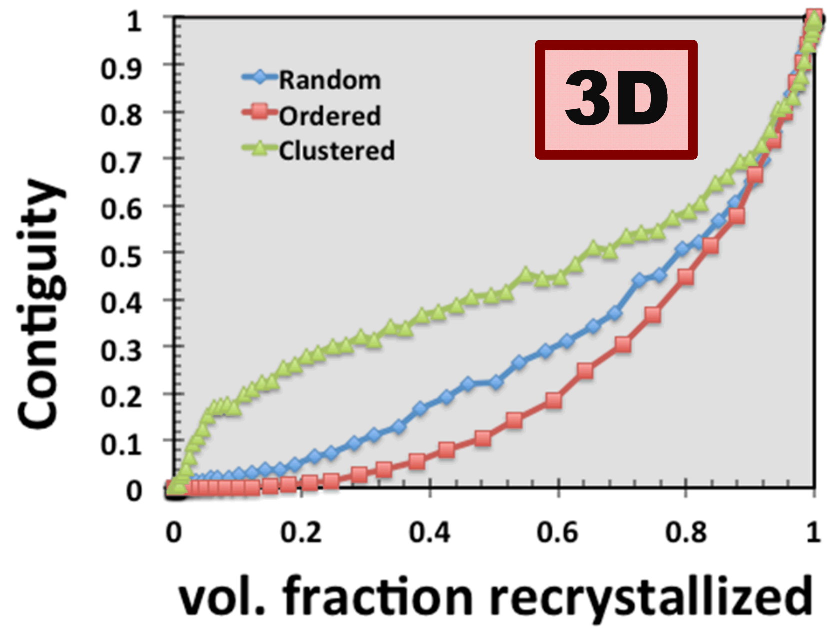
$$C_{\alpha\alpha} = \frac{2(S_v)_{\alpha\alpha}}{2(S_v)_{\alpha\alpha} + (S_v)_{\alpha\beta}}$$

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



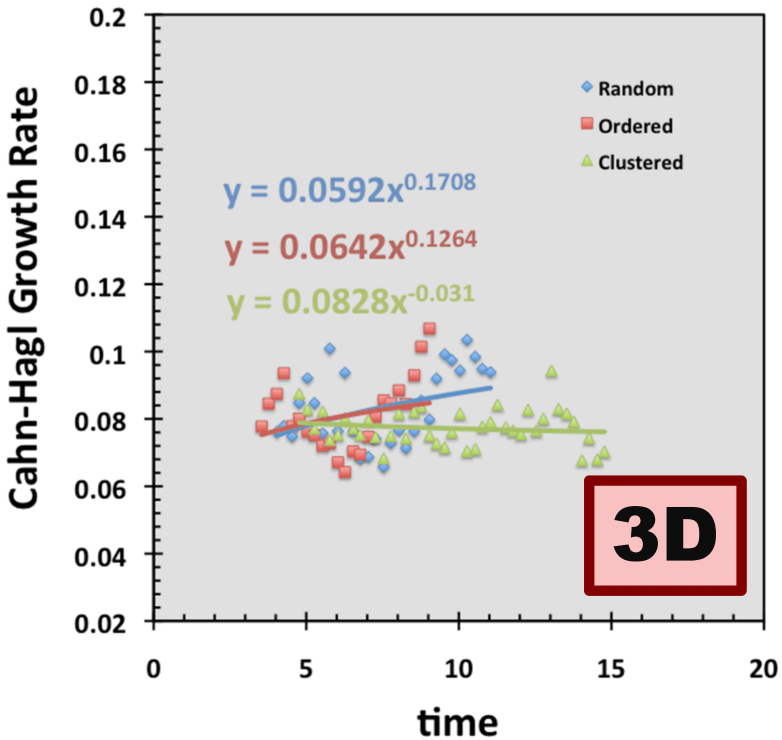


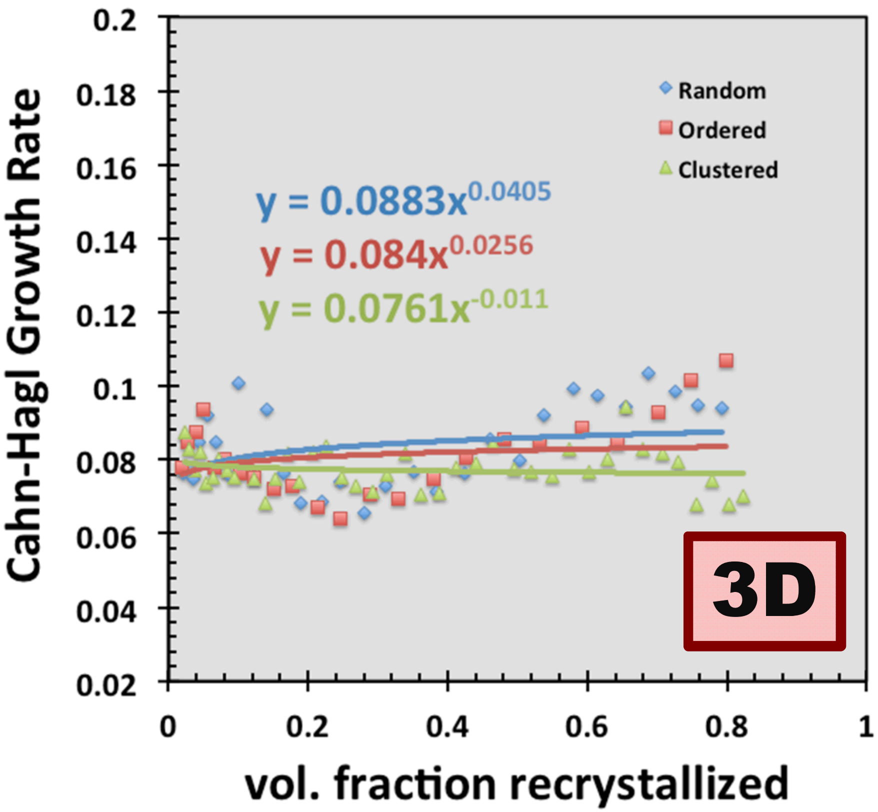
P. R. Rios, L. O. Pereira, F. F. Oliveira, W. L. S. Assis and J. A. Castro: *Acta Mat.*, 2007, vol. 55 pp. 4339-48.



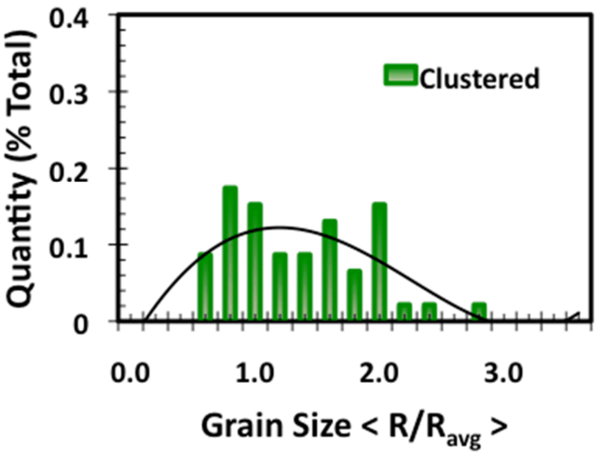
Cahn-Hagel Growth Rate

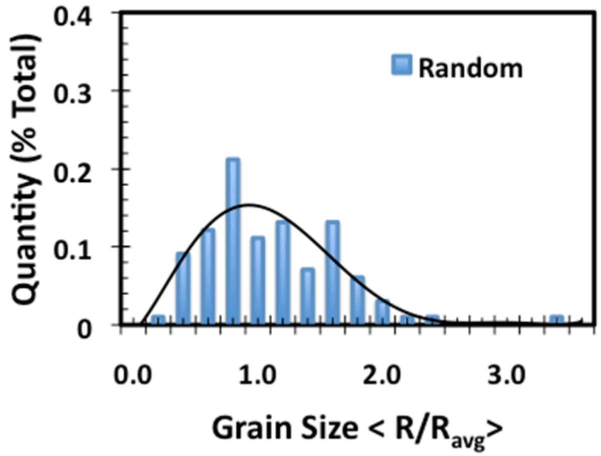
$$G_{Cahn-Hagel} = \left[\frac{1}{S_V}\right] * \left[\frac{dV_V}{dt}\right]$$

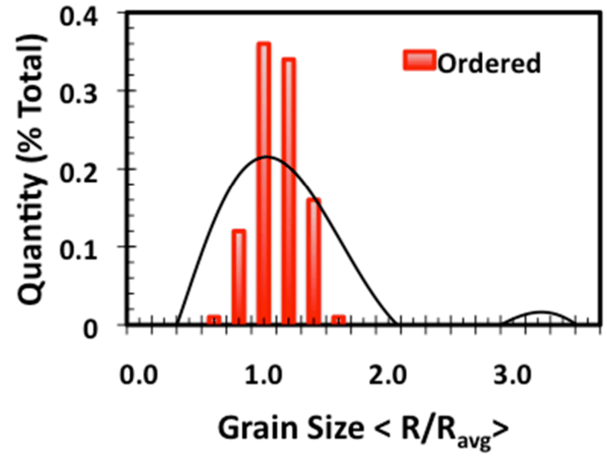




Grain Size Distributions







Coefficient of variation (CV)

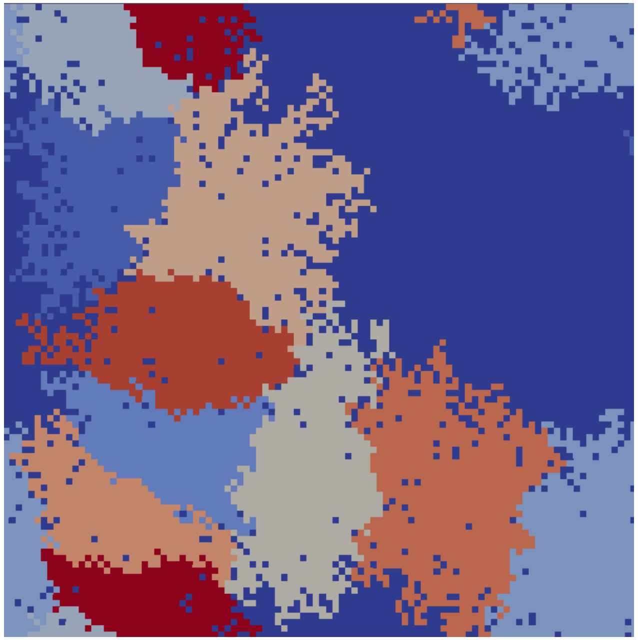
$$CV = \frac{\sigma}{\mu} = \frac{st.\ deviation}{mean}$$

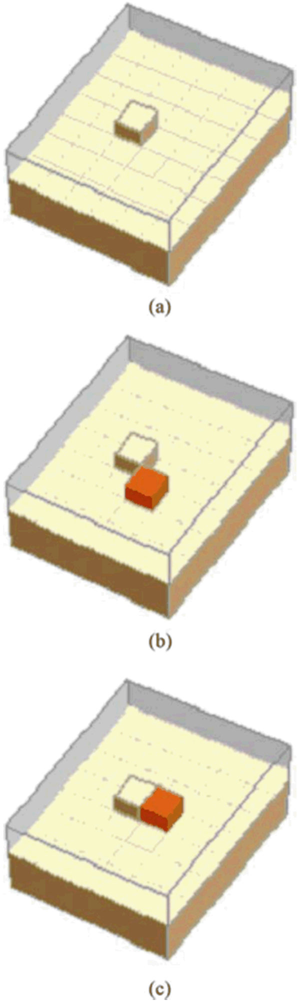
Provides extent of variability in relation to the mean of a population

	Clustered		Random		Ordered	
	R_{avg}	c.v.	R_{avg}	c.v.	R_{avg}	c.v.
0.10 V_v	401	0.46	244	0.32	260	0.26
0.50 V_v	1935	0.56	1273	0.34	1234	0.14
1.00 V_v	3906	0.71	2525	0.55	2499	0.18

Future Work

- Initial work shows enhanced surface roughness when employing three dimensions. This artifact has been denoted as “the model-lattice effect” by other investigators.





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

Summary

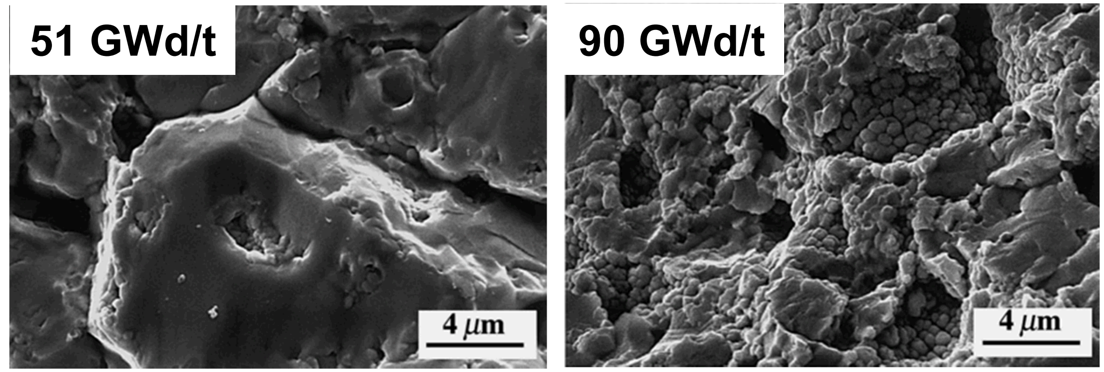
- The kMC-C.A. hybrid model viably mimics static recrystallization behavior in both 2 and 3 dimensions.
- The hybrid model represents a readily deployable methodology modeling recrystallization in simple systems and tracking microstructural evolution inclusive of;
  - interfacial surface areas,
  - KJMA exponents,
  - contiguity,
  - Cahn-Hagel growth rate
- While 3d simulations exhibit enhanced roughening, tracked features show reasonable agreement with trends previously identified by Rios et al., Marx et al. and Vandermeer

Questions

High Burn-Up Structure I

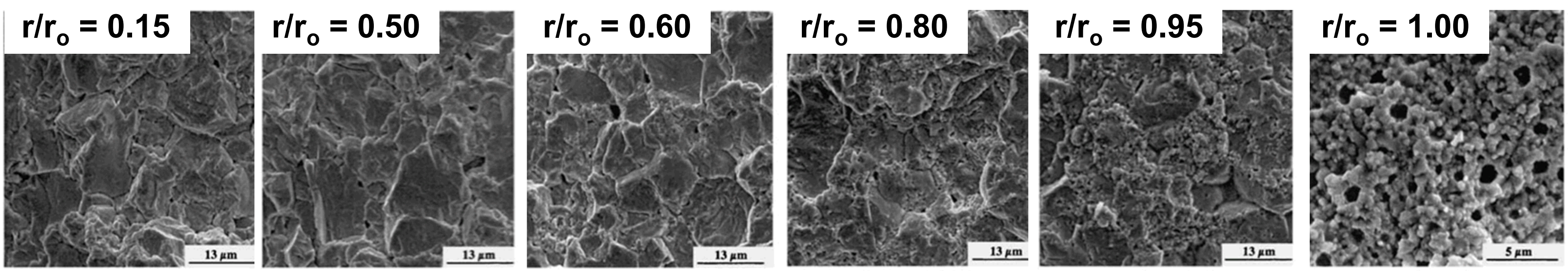
Sandia National Laboratories

- **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**



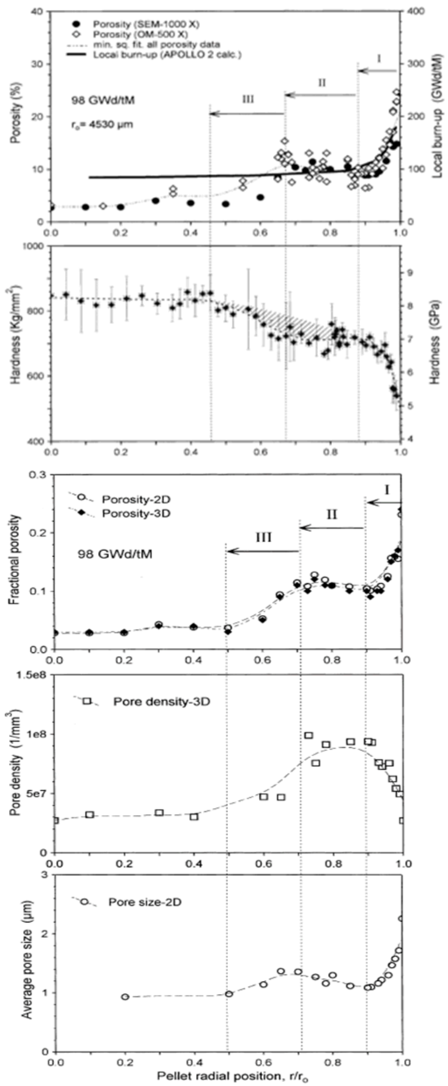
*Une, et. al, **JNM** vol. 288, 2001*

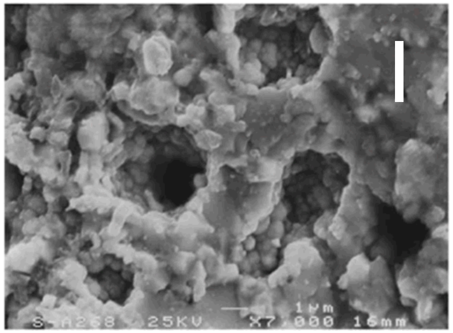
- **Since burn-up correlates with radial position recrystallization is largely absent as r/r_o decreases**

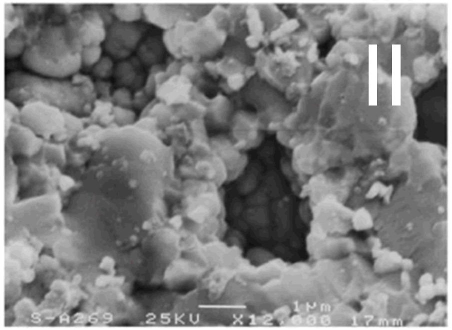


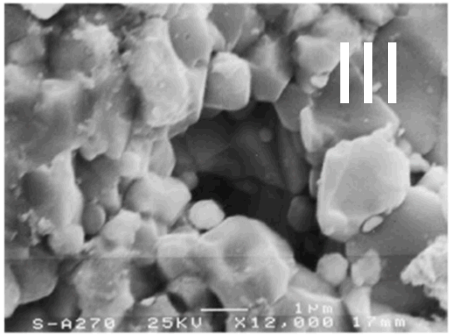
*Manzel & Walker, **JNM** vol. 301, 2002*

High Burn-Up Structure II





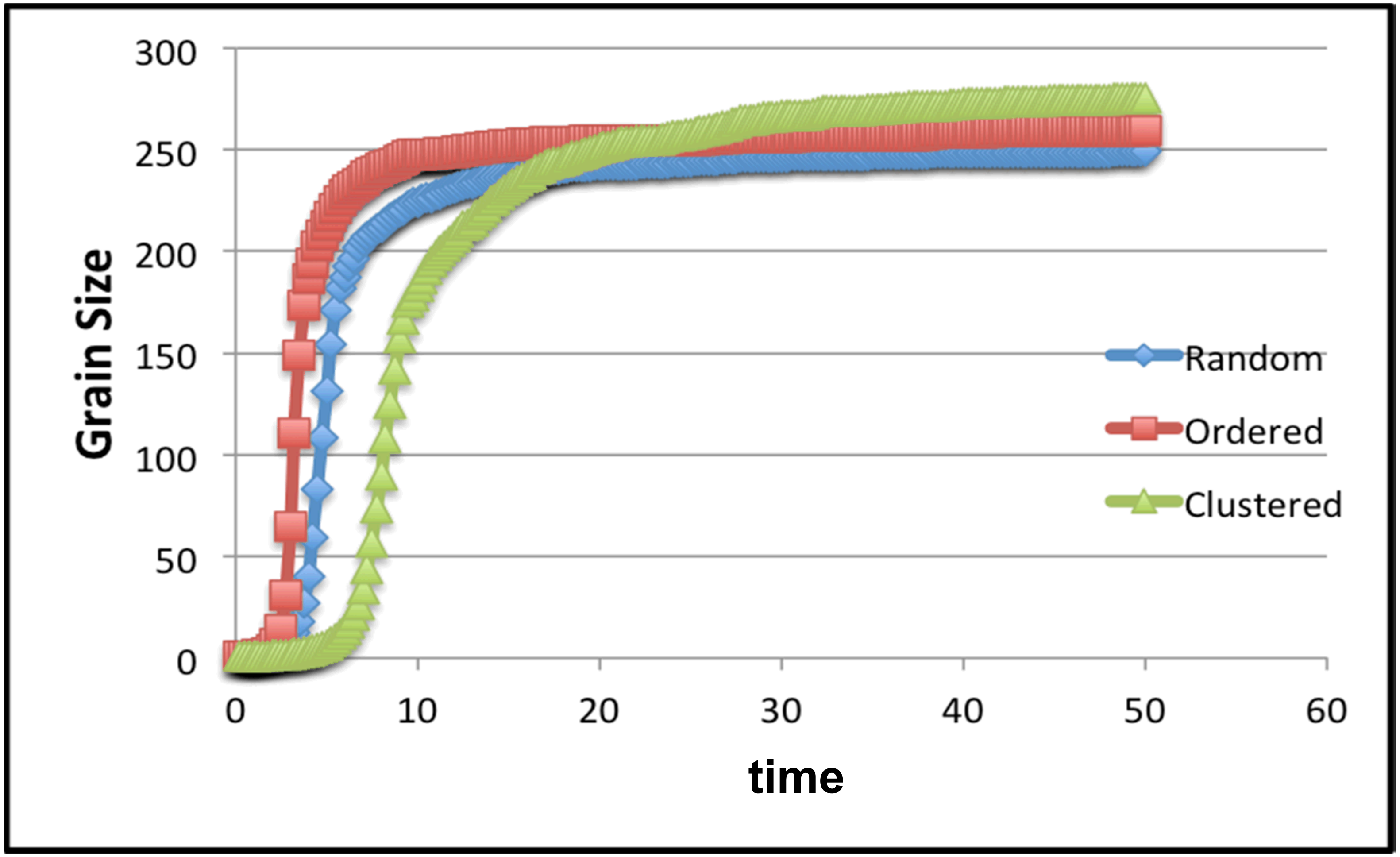




- **Understanding the rim effect is important**
  - **Effects fuel performance (thermal conductivity, fission product distributions, …)**
  - **Effects mechanical properties during storage and transportation**
  - **Modifies the separation processes for fuel recycling.**
- **Various aspects of the evolutionary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

*J. Spino et al., **JNM** vol. 354, 2006*

Grain Size


Grain Size
300
250
200
150
100
50
0
0
10
20
30
40
50
60
time
Random
Ordered
Clustered

Cumulative Frequency Distributions