Multiscale Simulation of Grain Growth and Deformation in Nanocrystalline Materials

D. Wolf

with

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Cluster Supercomputer Using Consumer Electronics

Interfacial Materials Group-
Materials Science Division, ANL

Hardware

Odin-I Beowulf Cluster

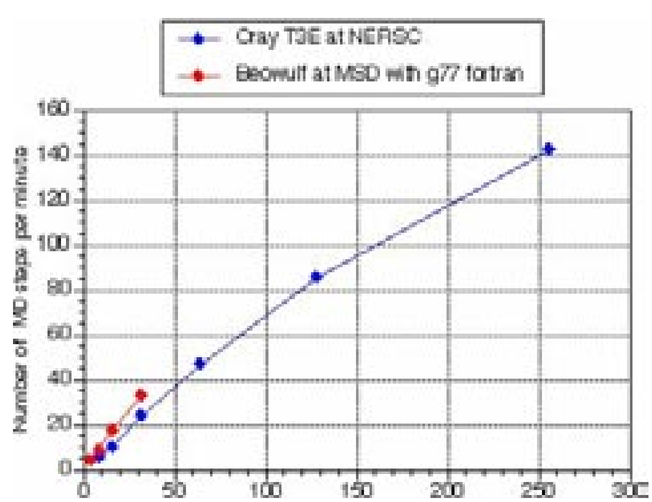
36 nodes - 450MHz Pentium III
(upgraded to 1GHz P III)

Odin-II Beowulf Cluster

100 nodes - 700MHz Pentium III

Performance

Odin II > Cray T3E 600MHz



Scientific Opportunity

Microstructure and its evolution are inherently difficult to characterize experimentally

→ **opportunity for an integrated simulation approach that incorporates all the distinct length and time scales of the underlying physics:**

- ***atomic- and electronic-level:*** **structure of grain boundaries and dislocations, their dynamical behavior and interactions**
- ***mesoscale:*** **spatial arrangement and dynamical behavior of microstructural "elements" (dislocations, grain boundaries, grain junctions, voids, precipitates, cracks,...)**
- ***continuum level:*** **Macroscopic materials behavior (phenomenological, continuum elasticity, constitutive laws...)**

Mechanical Properties of Polycrystalline Materials:
An Integrated Simulation Approach

Microstructurally designed materials are important in mar technologies...

- **high-temperature structural ceramics for aerospa applications**
- **light-weight aluminum alloys for fuel-efficient, cl automobiles**
- **thermal-barrier coatings for turbine engines**

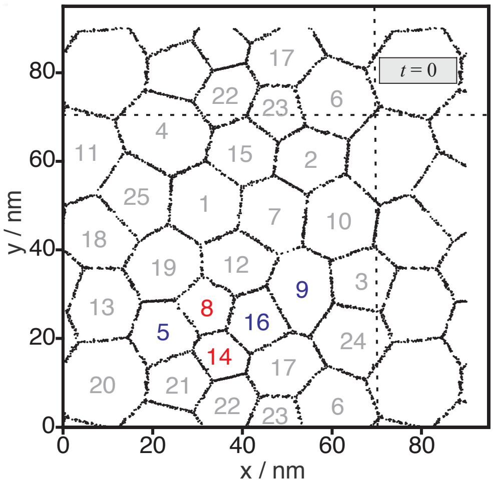
→ ***Microstructural control enables***

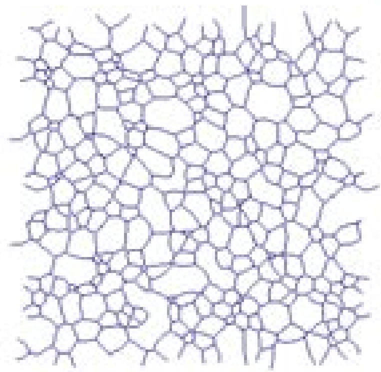
- **processing of inherently brittle materials (e.g., by superplastic forming)**
- **tailoring of microstructure-sensitive materials properties**

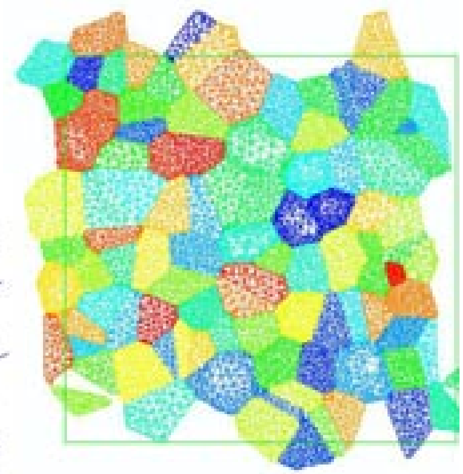
Mechanical properties of polycrystalline materials are controlled by the dynamical behavior and interaction among dislo-cations, grain boundaries, grain junctions voids, cracks etc.

Multiscale Simulation of Microstructural Evolution @ANL

Atomistic → Mesoscale ← Finite element







Newton's Law

Principle of virtual-power dissipation

Continuum level

Goal: Continuum simulations based on fundamental understanding of GB physics

OUTLINE

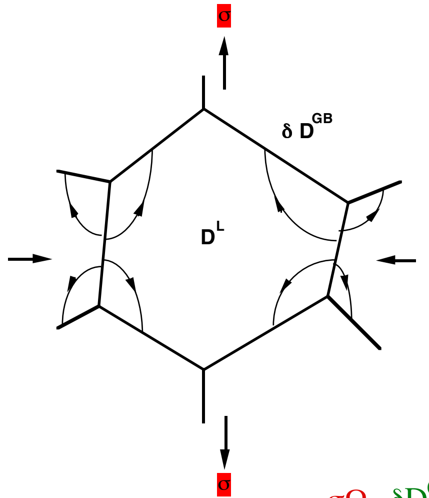
- *High-temperature deformation of nanocrystalline materials*
  - **High strain rates in MD simulations are meaningful!**
  - **Unique capability of computer simulation to consider idealized microstructures**
  - **Enables deconvolution of the interplay between various processes**

- *Atomic-level simulation of grain growth*
  - **Curvature-driven GB migration**
  - **Grain coalescence by coordinated grain rotations speeds up growth rate**
  - **Rotation rate ~ d^{-4}**

- *Mesoscale simulation of grain growth*
  - **Viscous law of motion for the grain boundaries and grains**
  - **Length scale given by grain size, time scale by GB mobility**
  - **Growth law, topology**

- *Ultimate goal: FEM simulations with microstructural materials input*

Grain-boundary diffusion creep



Coble (1963): $\dot{\varepsilon} = 47 \frac{\sigma\Omega}{kT} \frac{\delta D^{GB}}{d^3}$

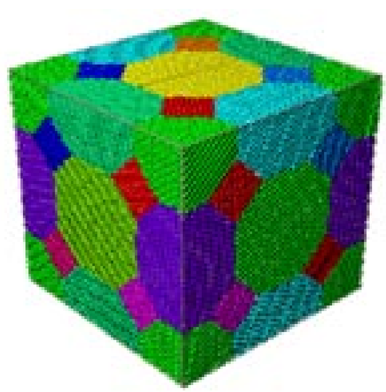
Gleiter, 1989: nc materials should deform via Coble creep, even at rather low temperatures (‘RT ductility’)

- Intrinsically brittle materials should become ductile if the grain size is only small enough
- No strain hardening
- Very high strain rates (> 10^7 s^{-1}) accessible byMD!
- Lu (Science 2000): Superplastyicity in nc Cu!

Grain-boundary diffusion creep in nanocrystalline Pd

(V. Yamakov et al., Acta Mat. 50, 2002, 61 ; P. Keblinski et al., Interface Sci. 6, 1998, 205)

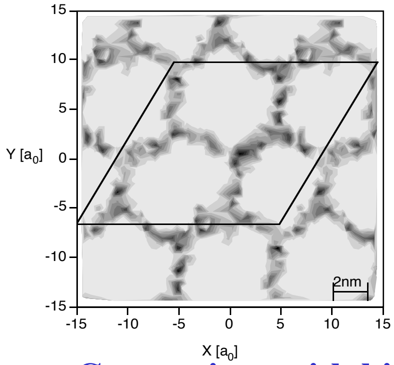
Idea: Design microstructure that is stable against grain growth!

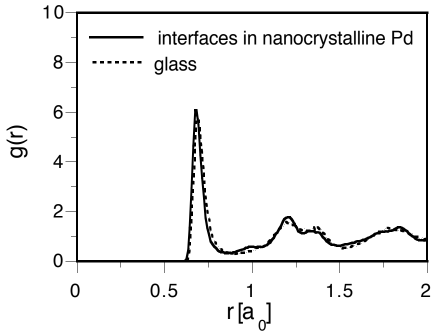


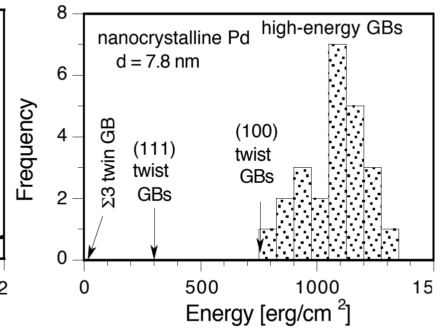
- 16 grains of identical shape and size arranged periodically on a bcc lattice
- Grain size: d = 3.8 - 15.2 nm (system size: 55,000 - 3.6 million atoms)
- Random grain orientations: only high-energy GBs (with fast, liquid-like self-diffusion at high T)
- T = 900 - 1300 K (T_m = 1500 K)
- Stress below dislocation-nucleation threshold stress

Grain Boundaries in Nanocrystalline Pd with Random Grain Orientations

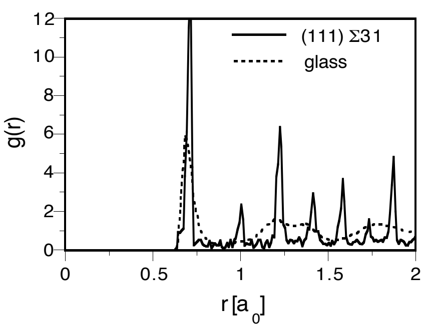
(P. Keblinski et al., Scripta Mat. 41,1999, 631)

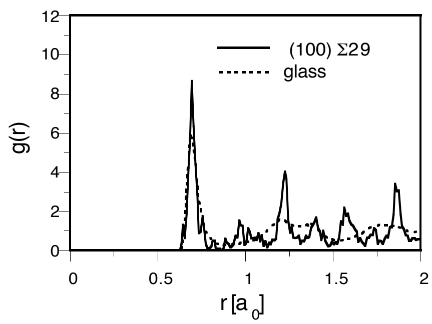


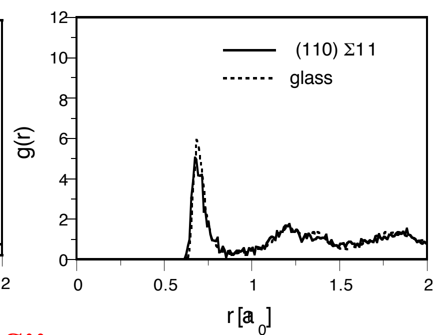




Comparison with bicrystalline GBs (or GBs in coarse-grained polycrystal):

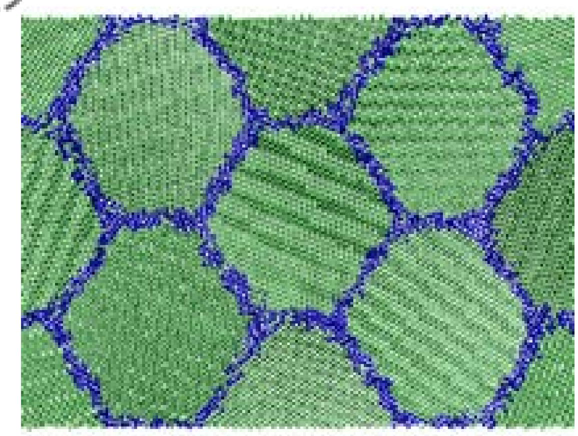






Qualitatively identical to Si!

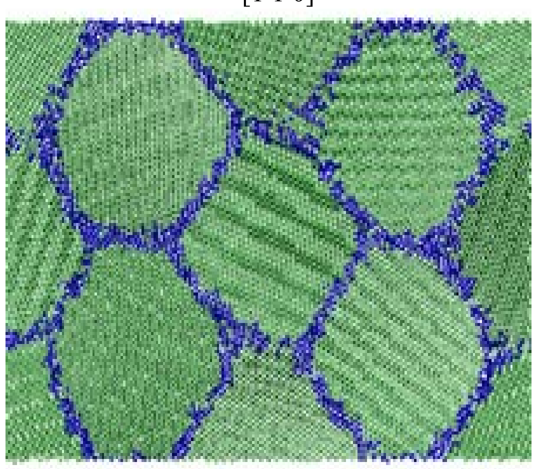
T=1200K



σ=0.4 GPa

11 ps.

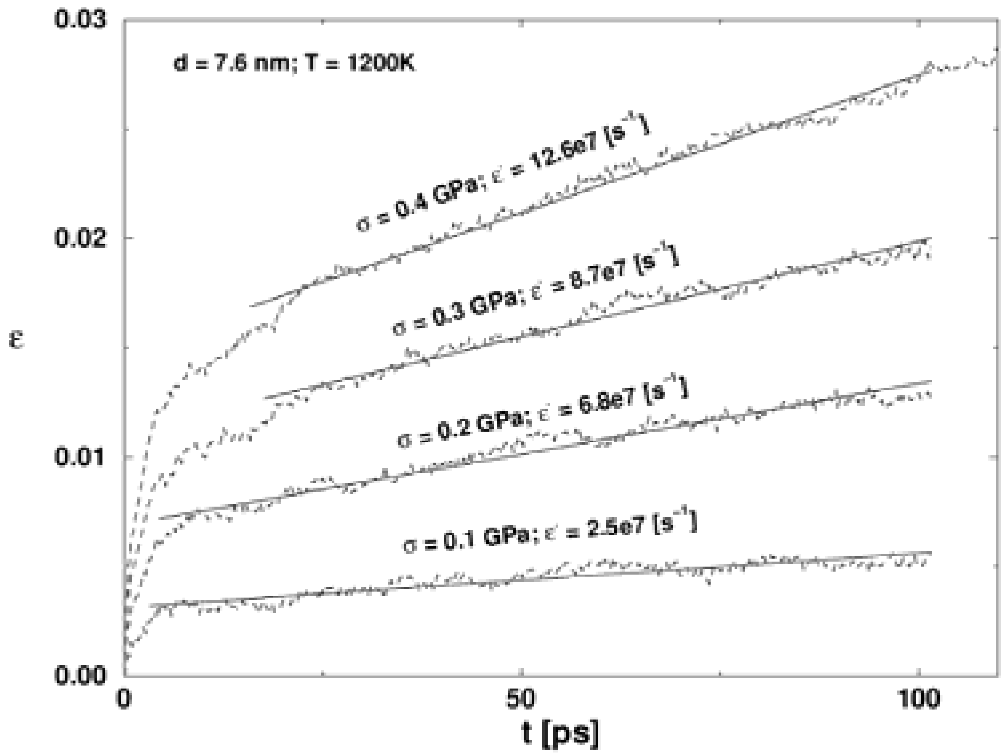
[1 1 0]



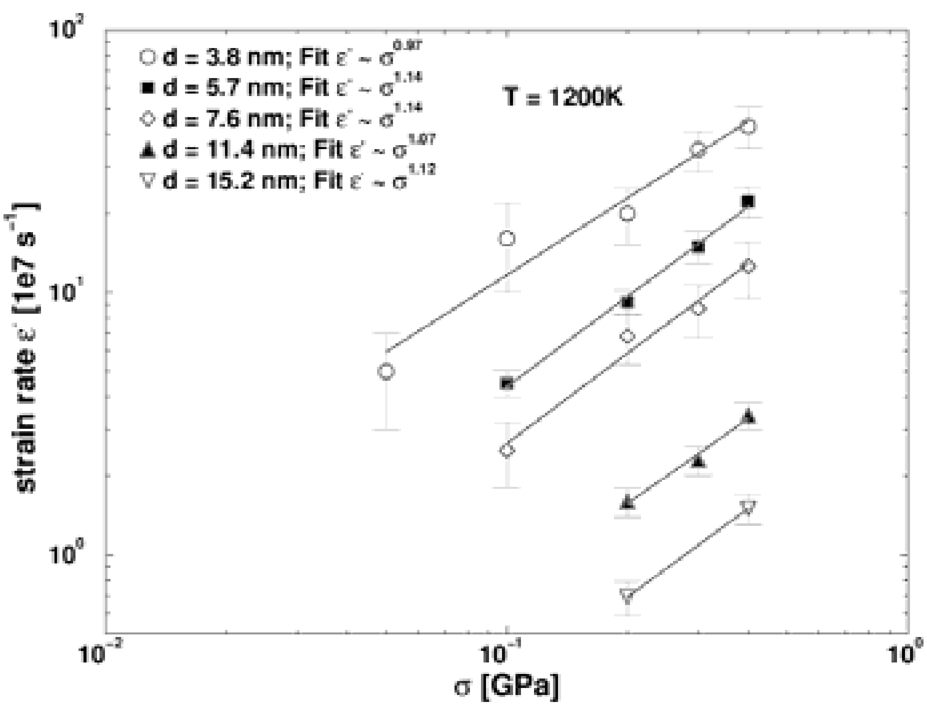
σ=0.4 GPa

82 ps

Steady-state creep under uniform tensile stress

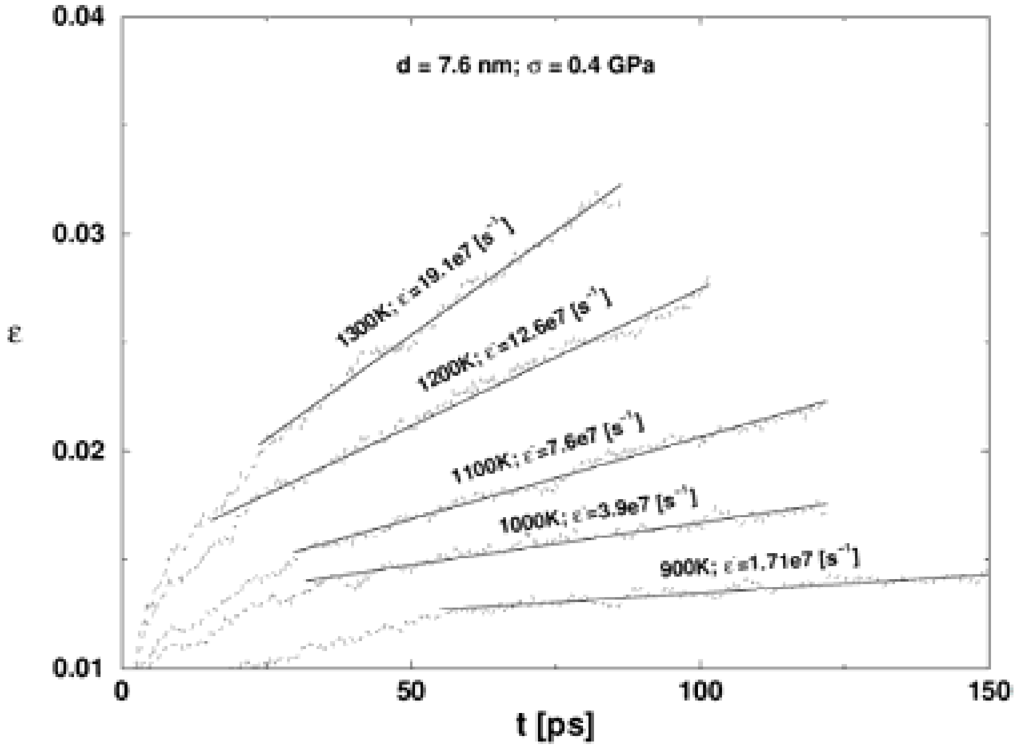


Strain rates are *linear* with applied stress!



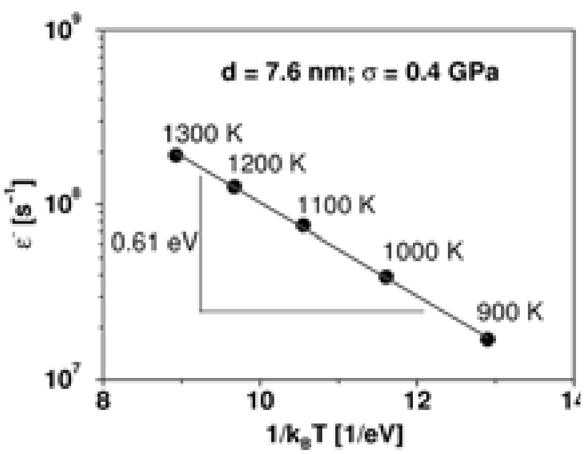
$$\dot{\varepsilon} = A\frac{\sigma\Omega_D}{k_B T}\frac{\delta_D D_{GB}}{d^3}$$

Temperature dependence of the creep rate

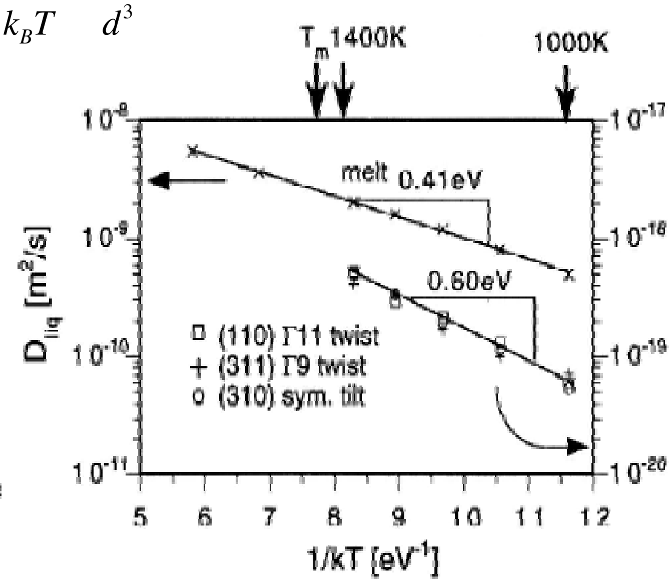


Activation energy of the creep rate

$$\dot{\varepsilon} = A\frac{\sigma\Omega_D}{k_B T}\frac{\delta_D D_{GB}}{d^3}$$



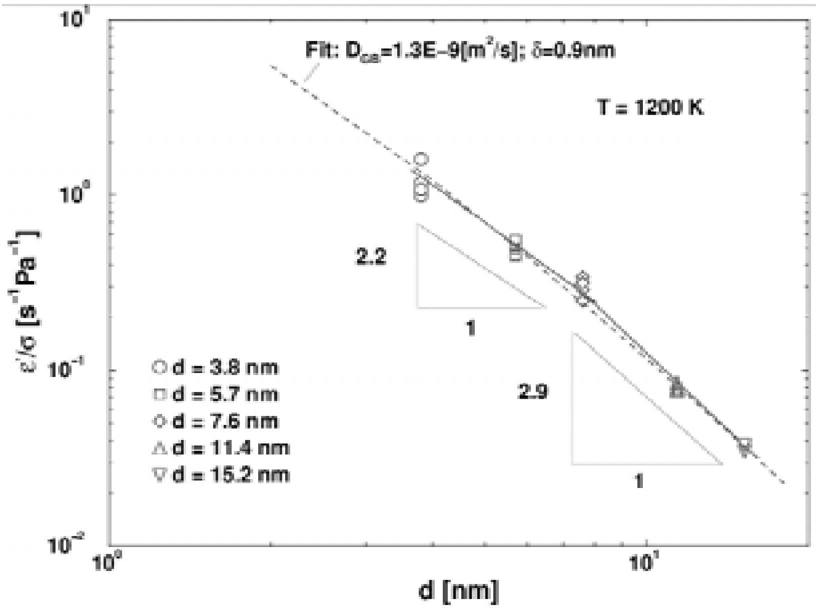
(V. Yamakov et al., Acta Mat. 50,2002, 61)



(P. Keblinski et al., Phil. Mag. A 79, 1999, 2735)

Identical to that for GB diffusion in high-energy bicrystalline GBs!

Grain-size dependence of the creep rate



$$\dot{\varepsilon} = A \frac{\sigma \Omega_D}{k_B T} \frac{\delta_D D_{GB}}{d^3}$$

Large grain size (d >> δ): creep rate ~ d^{-3} (Coble!)
Small grain size: (d ≈ δ): creep rate ~ d^{-2}

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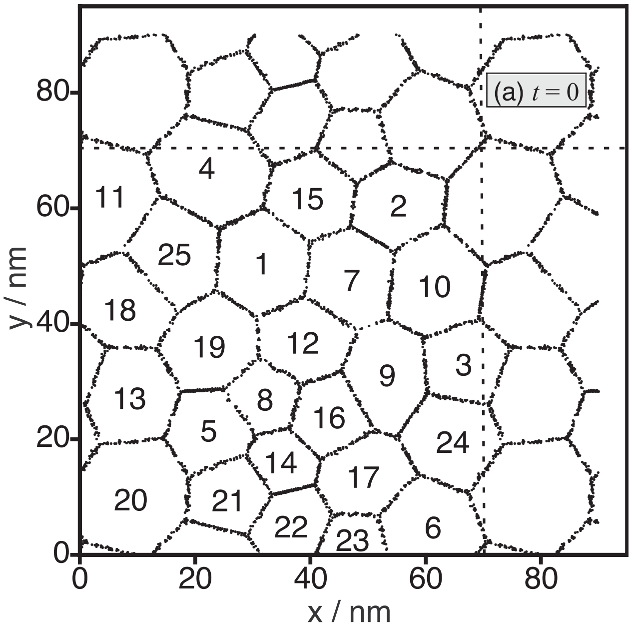
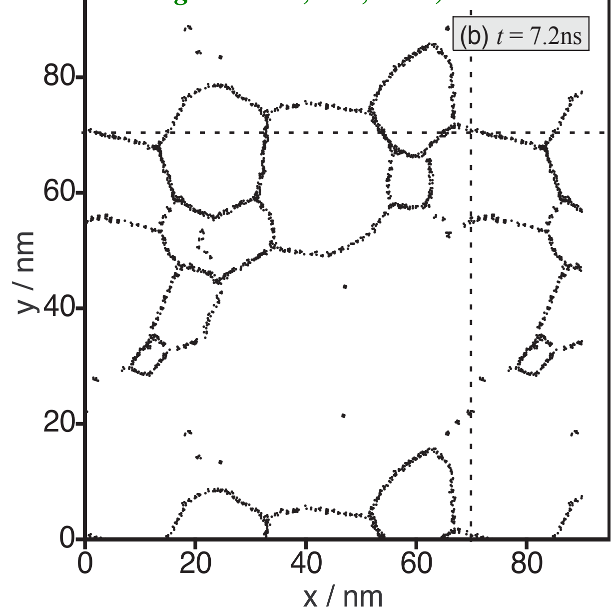
Grain growth in a <100> textured Pd polycrystal

(A. Haslam et al., *Mat. Sci & Engin.* A 318, 293, 2001)





t=0

<100> columnar microstructure

25 grains, d=15 nm, Θ_{min} ~14.9°,

~400,000 atoms

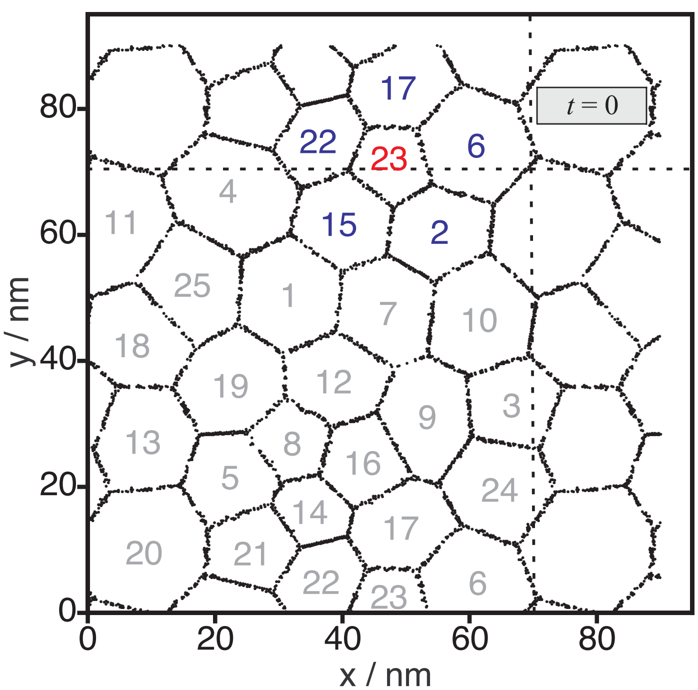
t=7.2 ns

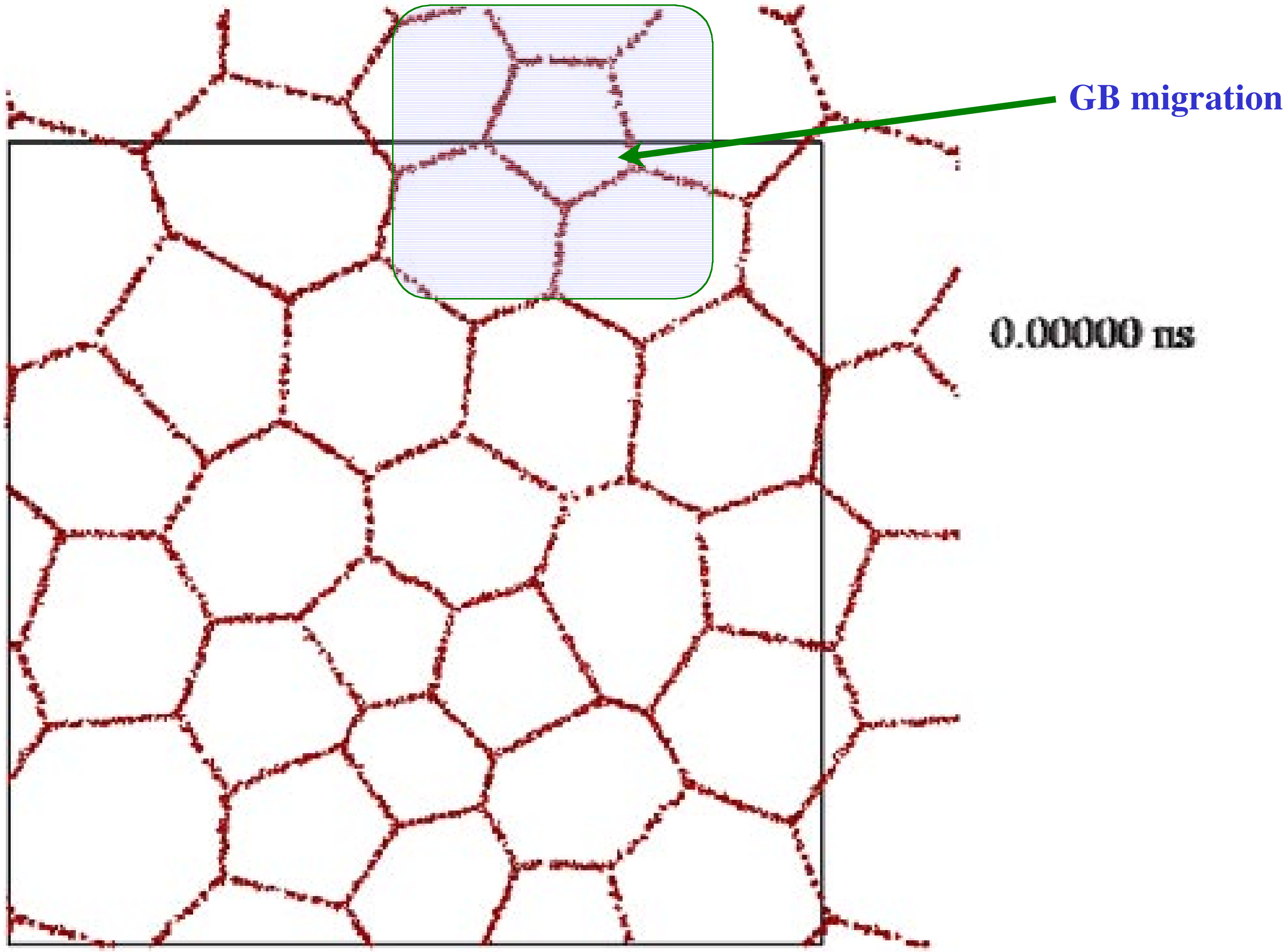
1.4 million MD time steps

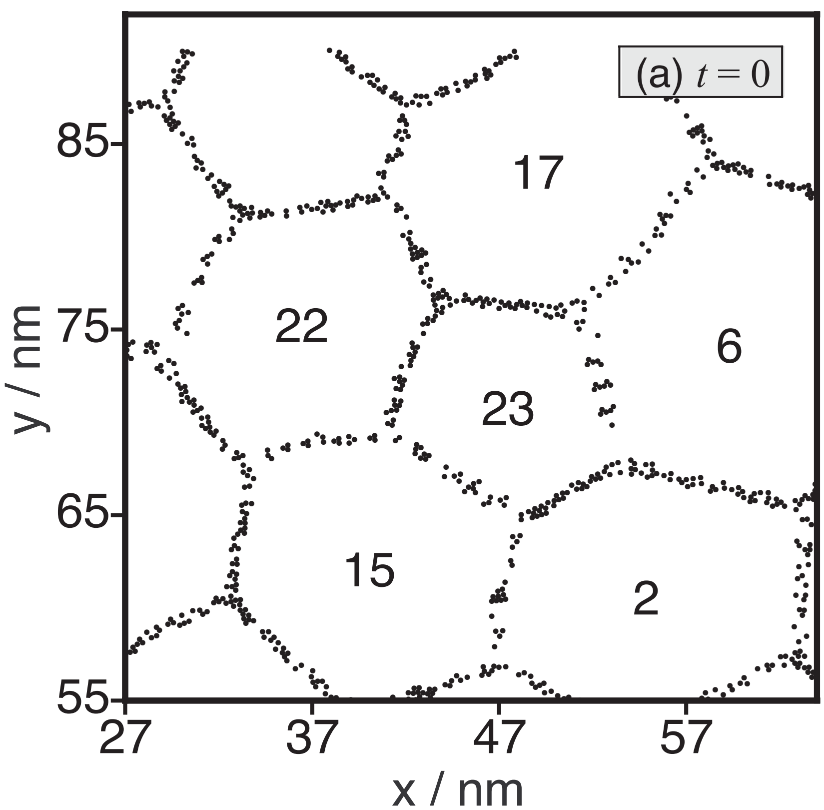
Pd (EAM) potential

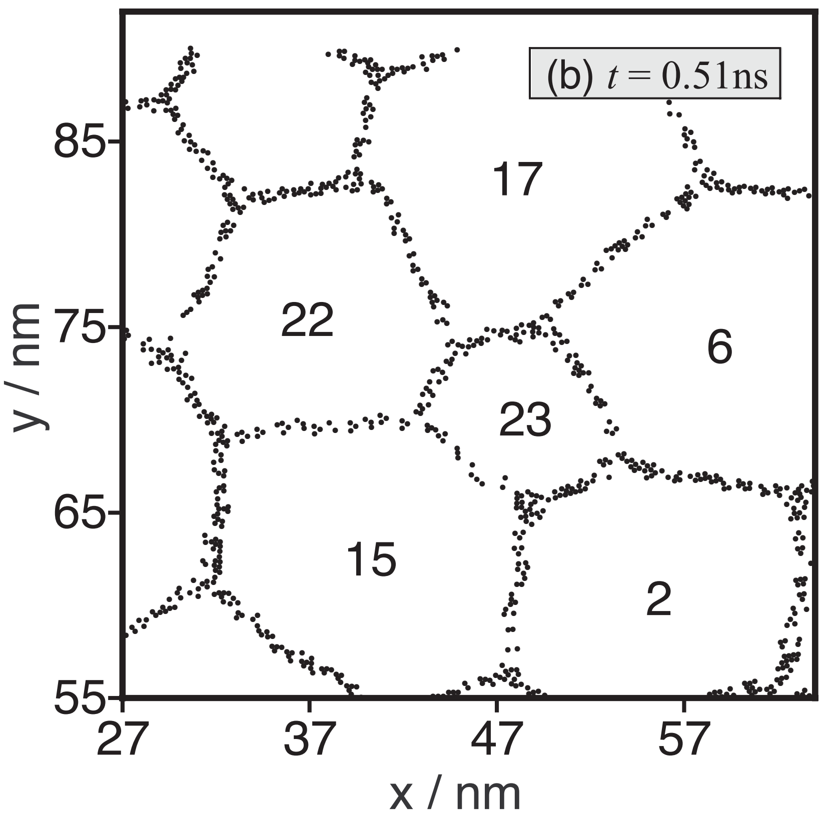
fully 3d physics

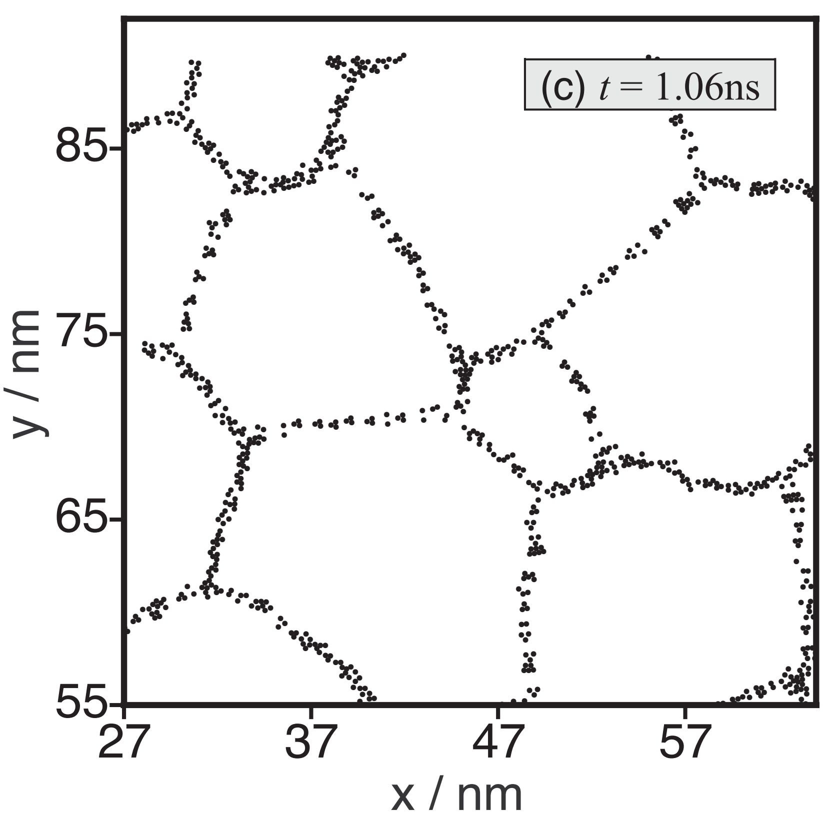
Curvature-driven grain-boundary migration

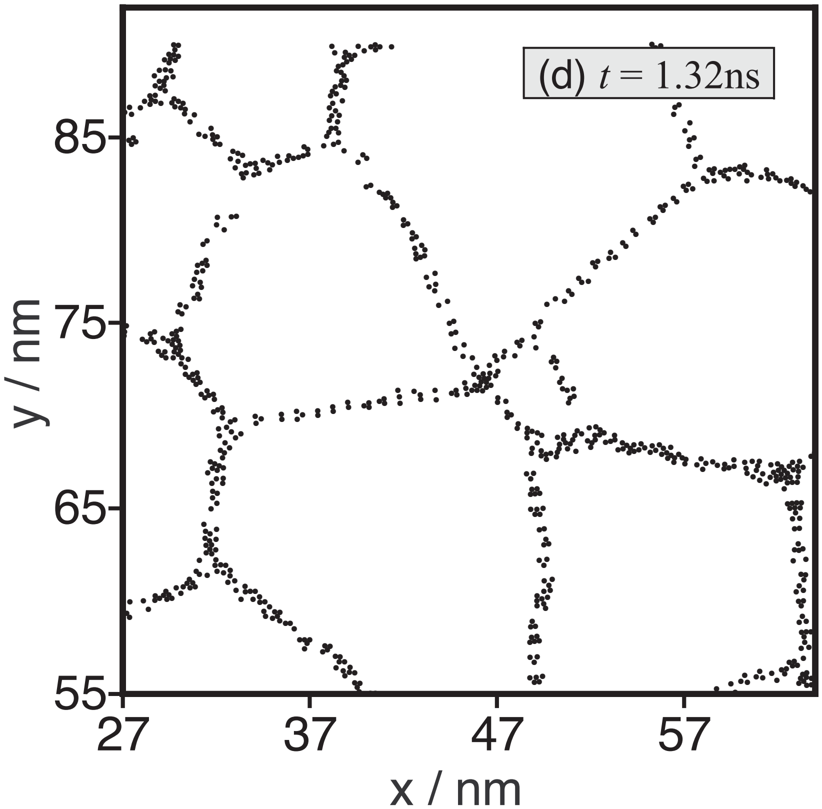



GB migration
0.00000 ns

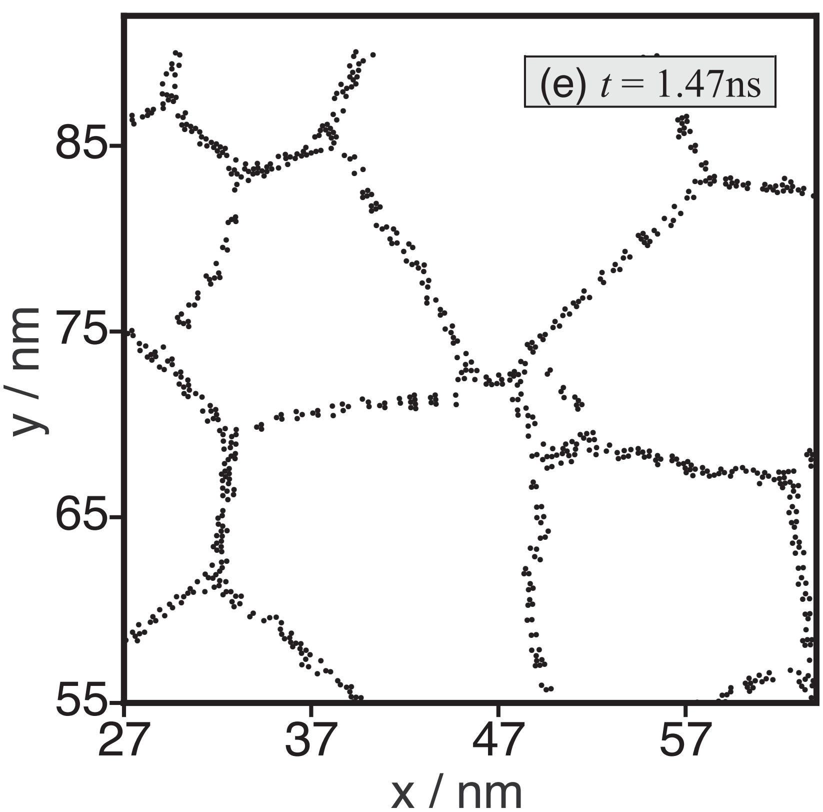

(a) t = 0
17
22
6
23
15
2
85
75
65
55
y / nm
27
37
47
57
x / nm


(b) t = 0.51ns
17
22
6
23
15
2
85
75
65
55
y / nm
27
37
47
57
x / nm

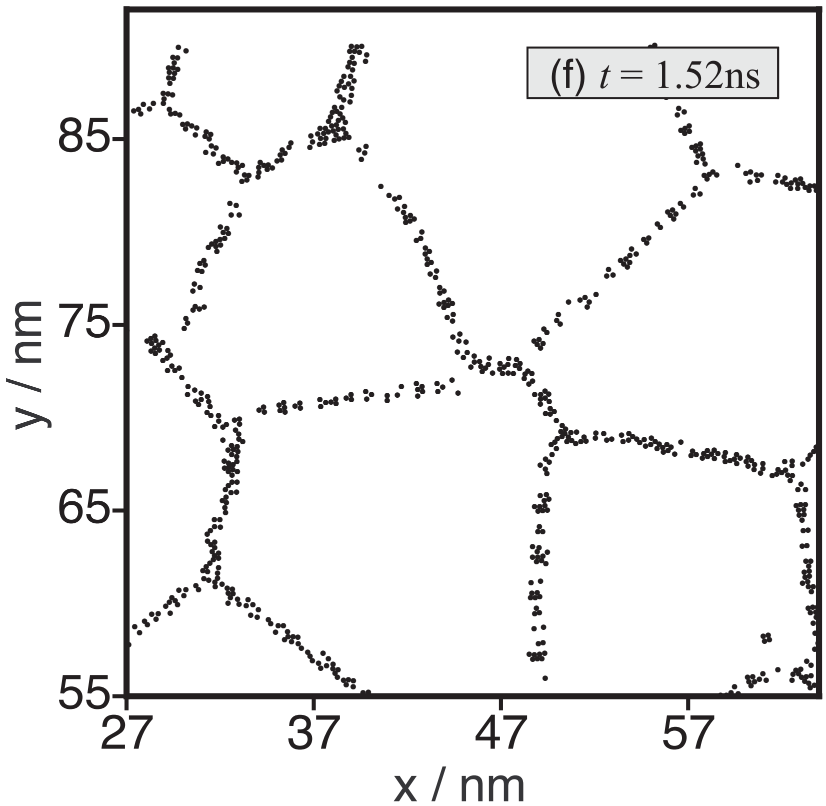

(c) t = 1.06ns
85
75
65
55
y / nm
27
37
47
57
x / nm



(d) t = 1.32ns
85
75
65
55
27
37
47
57
y / nm
x / nm

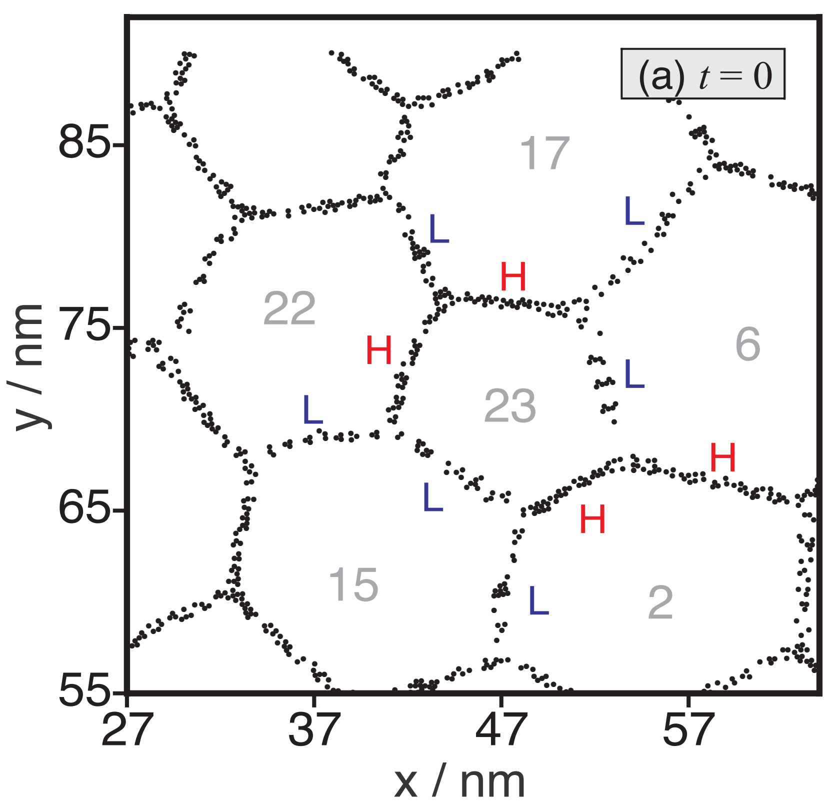


(e) t = 1.47ns
85
75
65
55
27
37
47
57
y / nm
x / nm

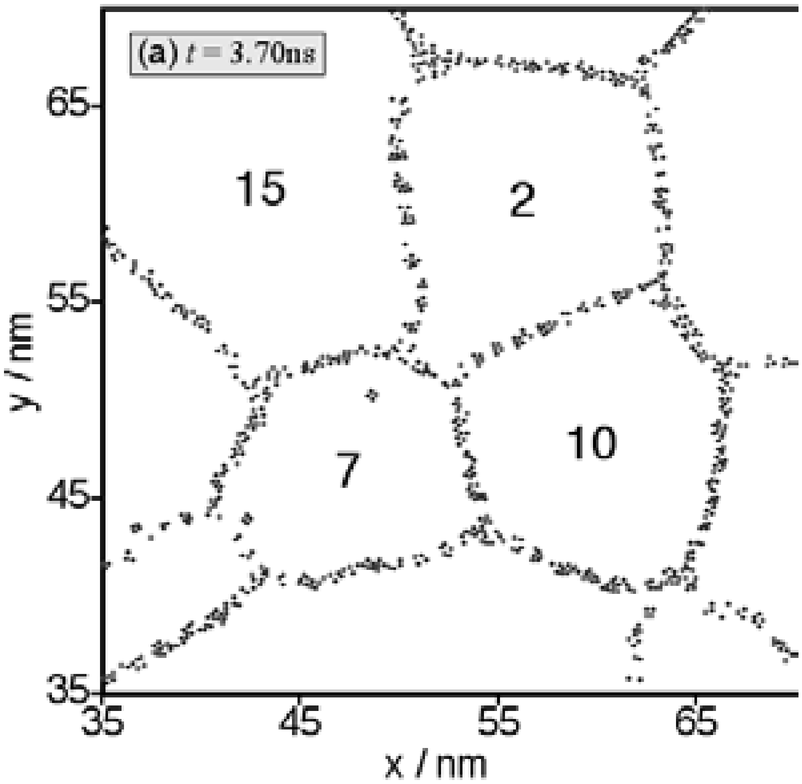


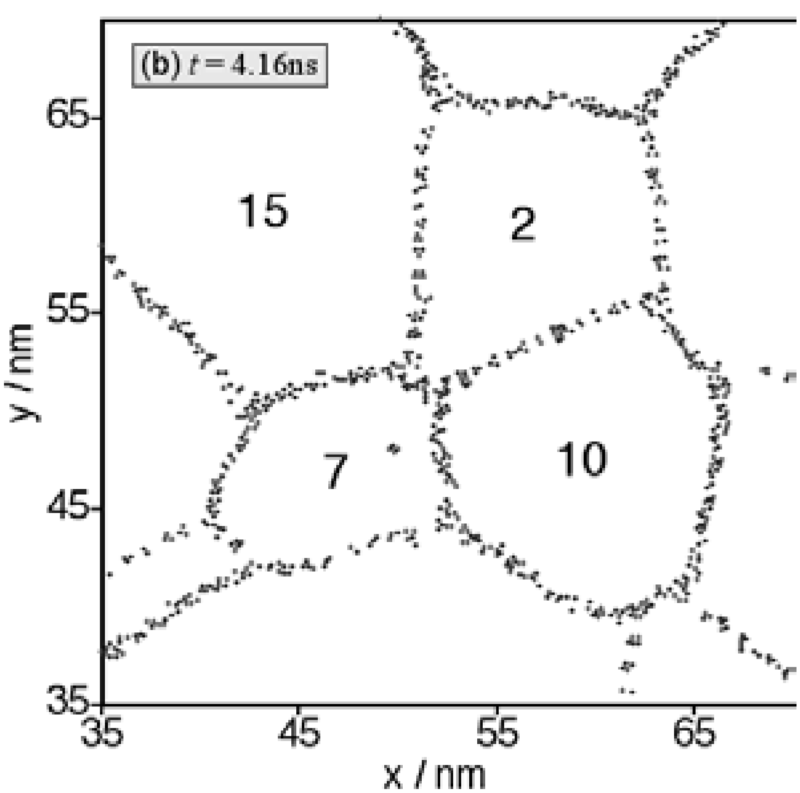
High-energy GBs disappear by GB migration

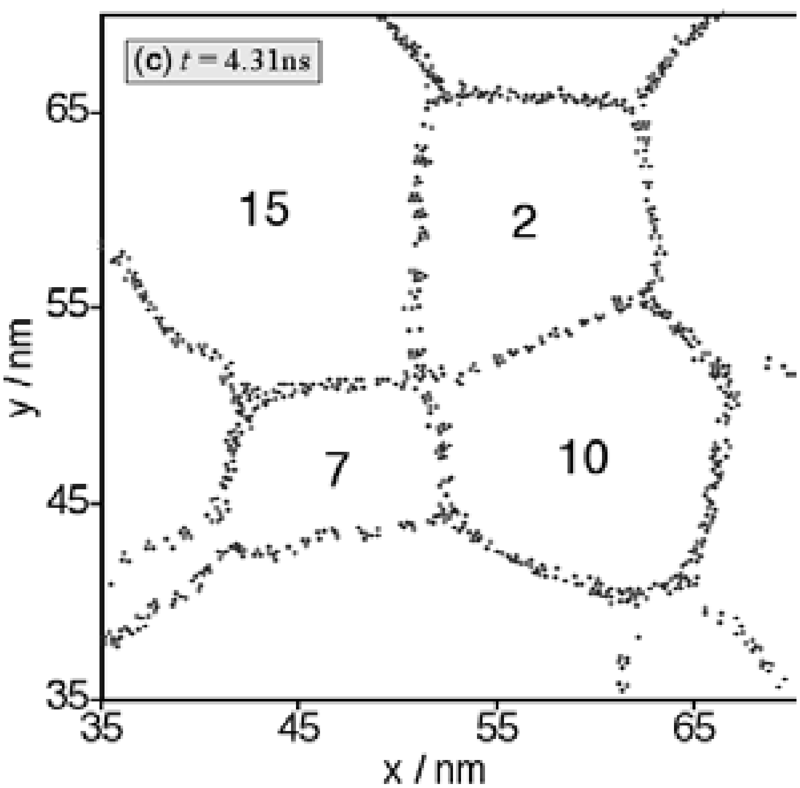
(A. Haslam et al., *Mat. Sci & Engin. A* 318, 293, 2001)

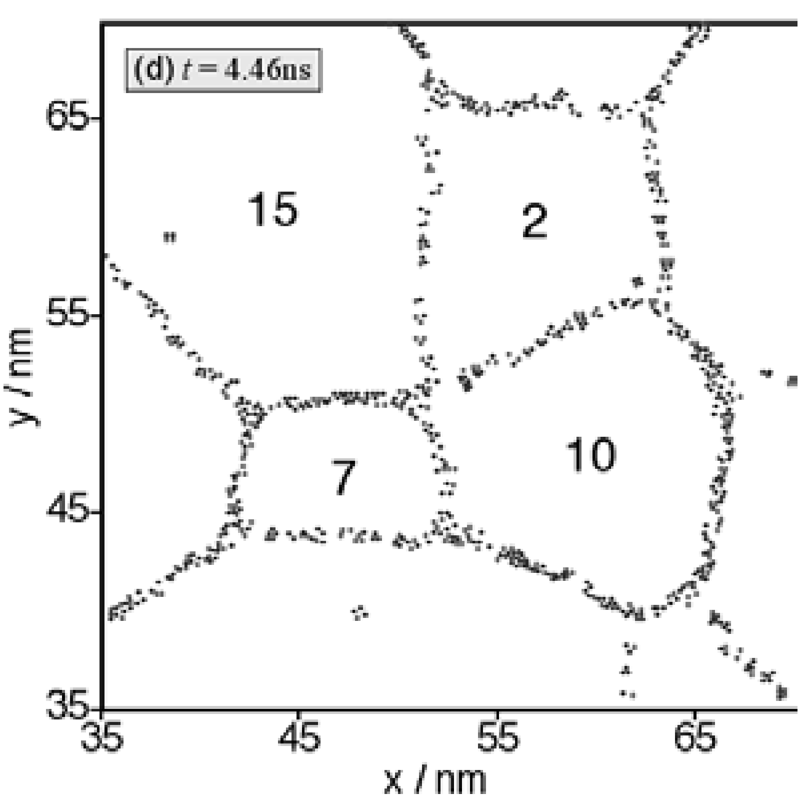


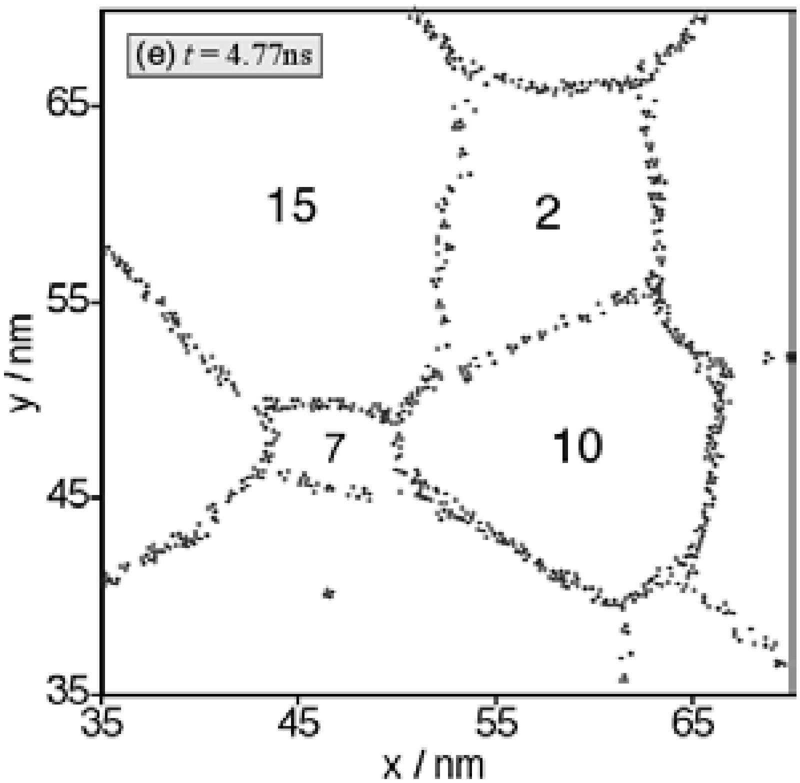
T1 SWITCHING PROCESS



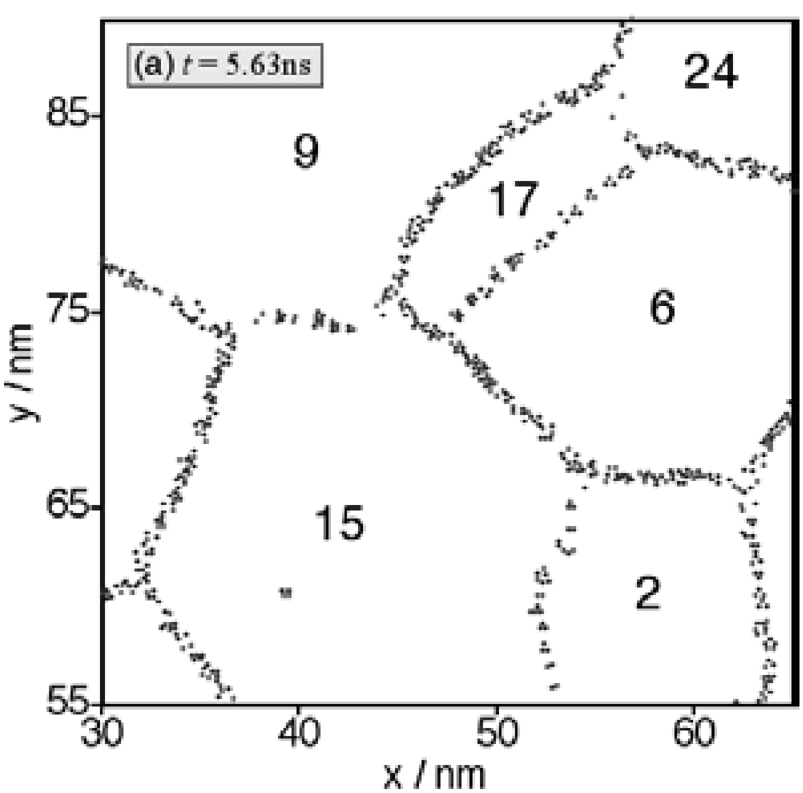


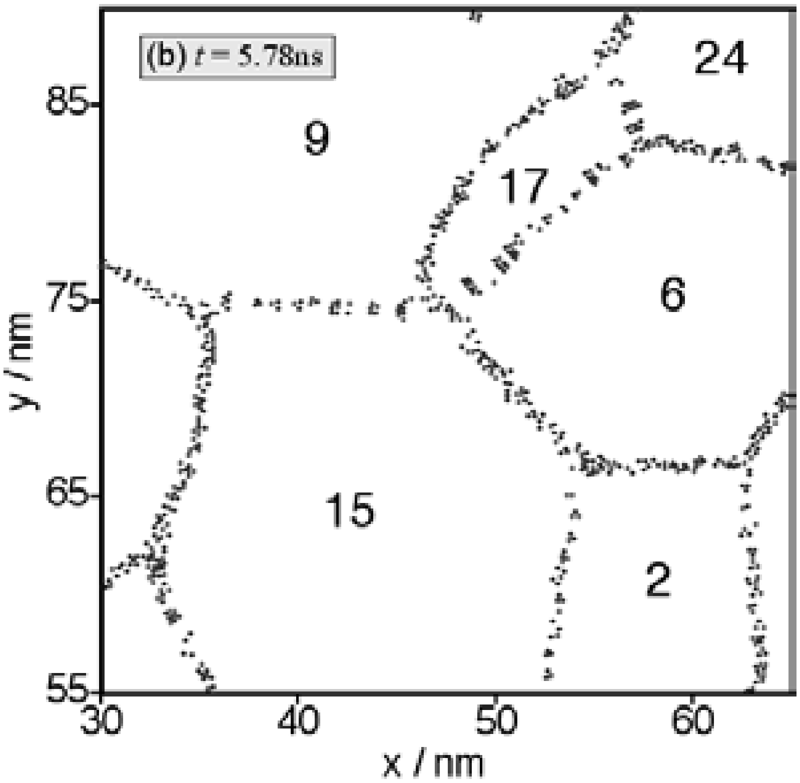

(c) t = 4.31ns
15
2
7
10
y / nm
x / nm
65
55
45
35
35
45
55
65

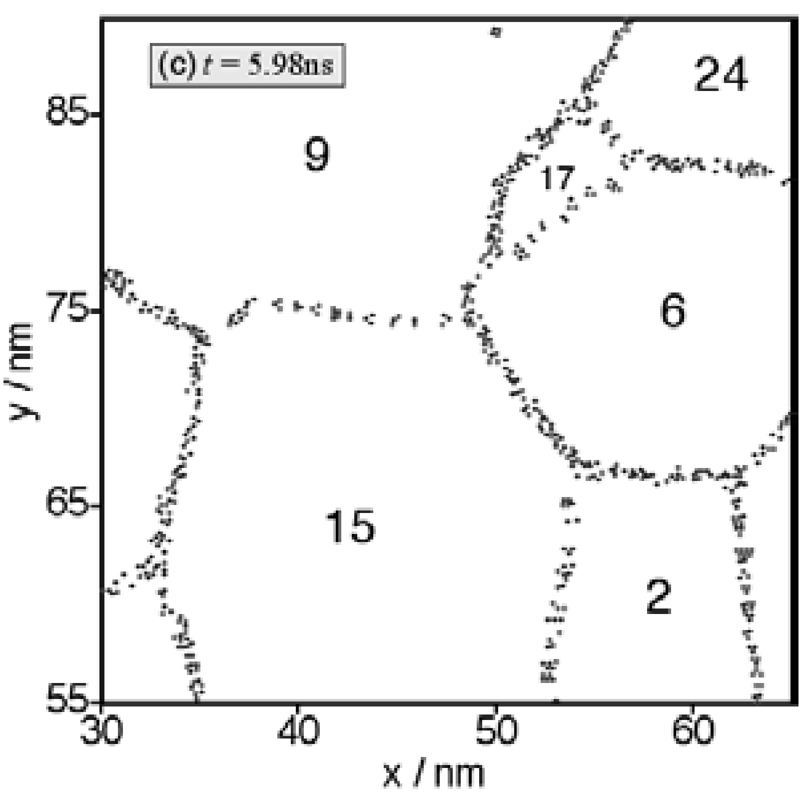

(d) t = 4.46ns
15
2
7
10
y / nm
x / nm
65
55
45
35
35
45
55
65

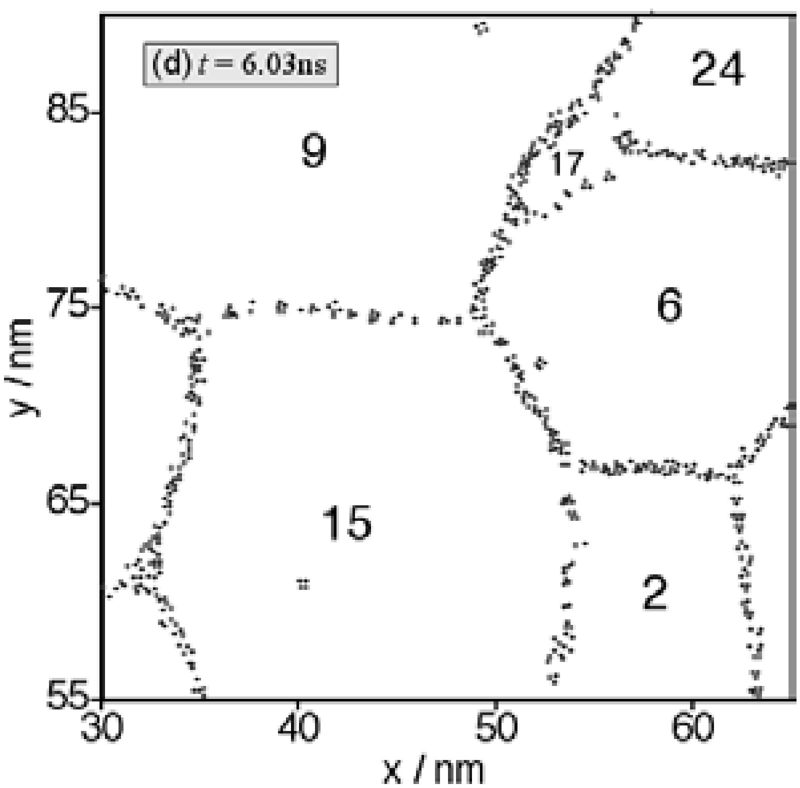


T1 SWITCH
triggering
T2 GRAIN DISAPPEARANCE

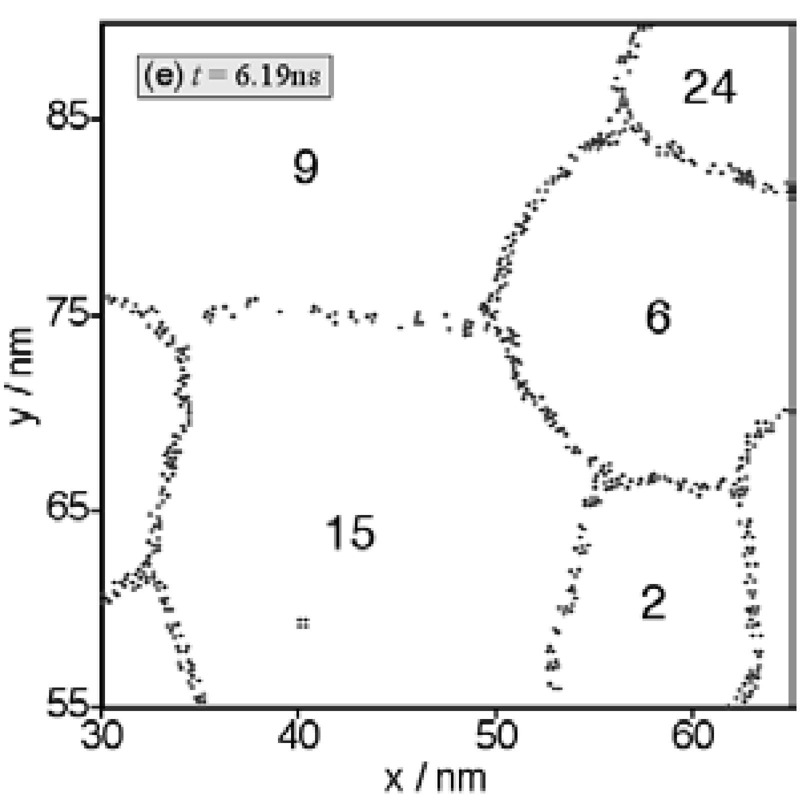



(b) t = 5.78ns
24
9
17
6
15
2
85
75
65
55
30
40
50
60
y / nm
x / nm


(c) t = 5.98ns
24
9
17
6
15
2
85
75
65
55
30
40
50
60
y / nm
x / nm



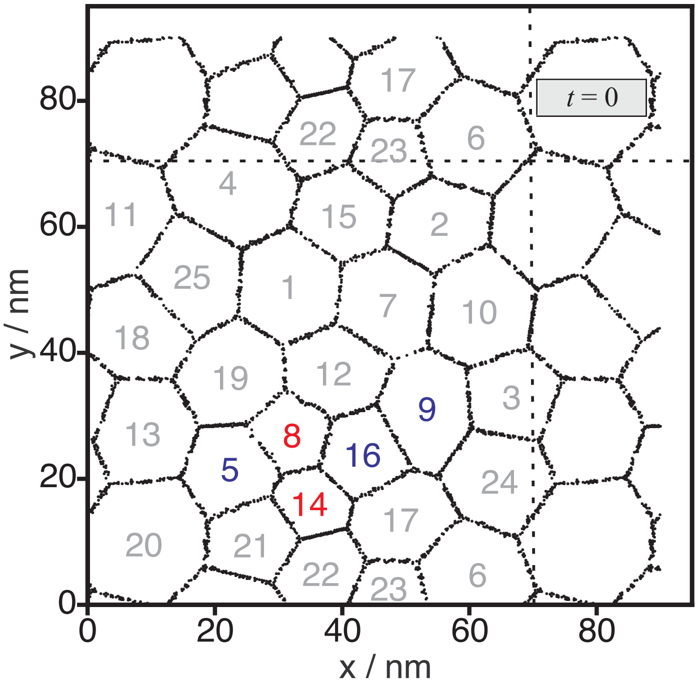
(d) t = 6.03ns
24
9
17
6
15
2
85
75
65
55
y / nm
30
40
50
60
x / nm

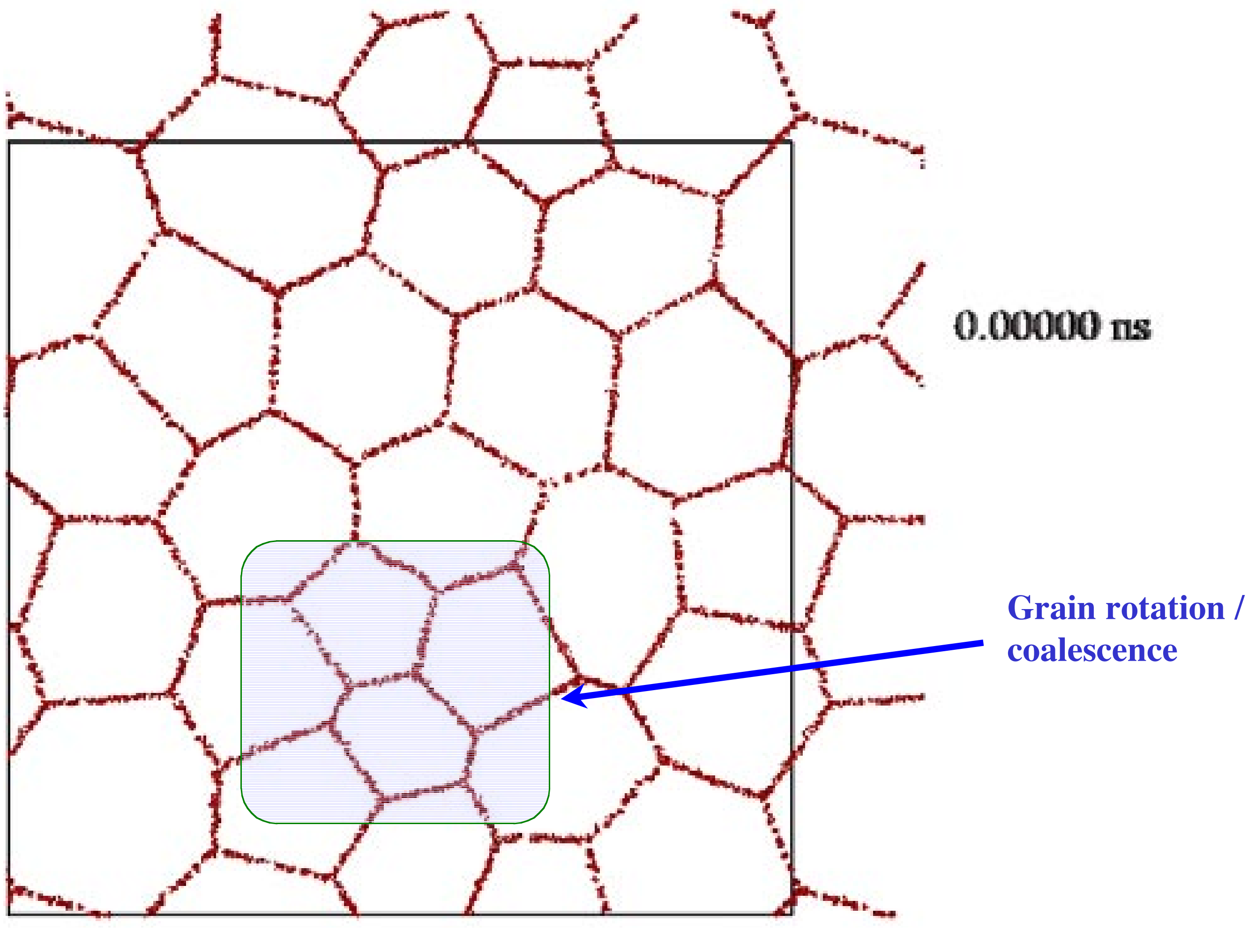


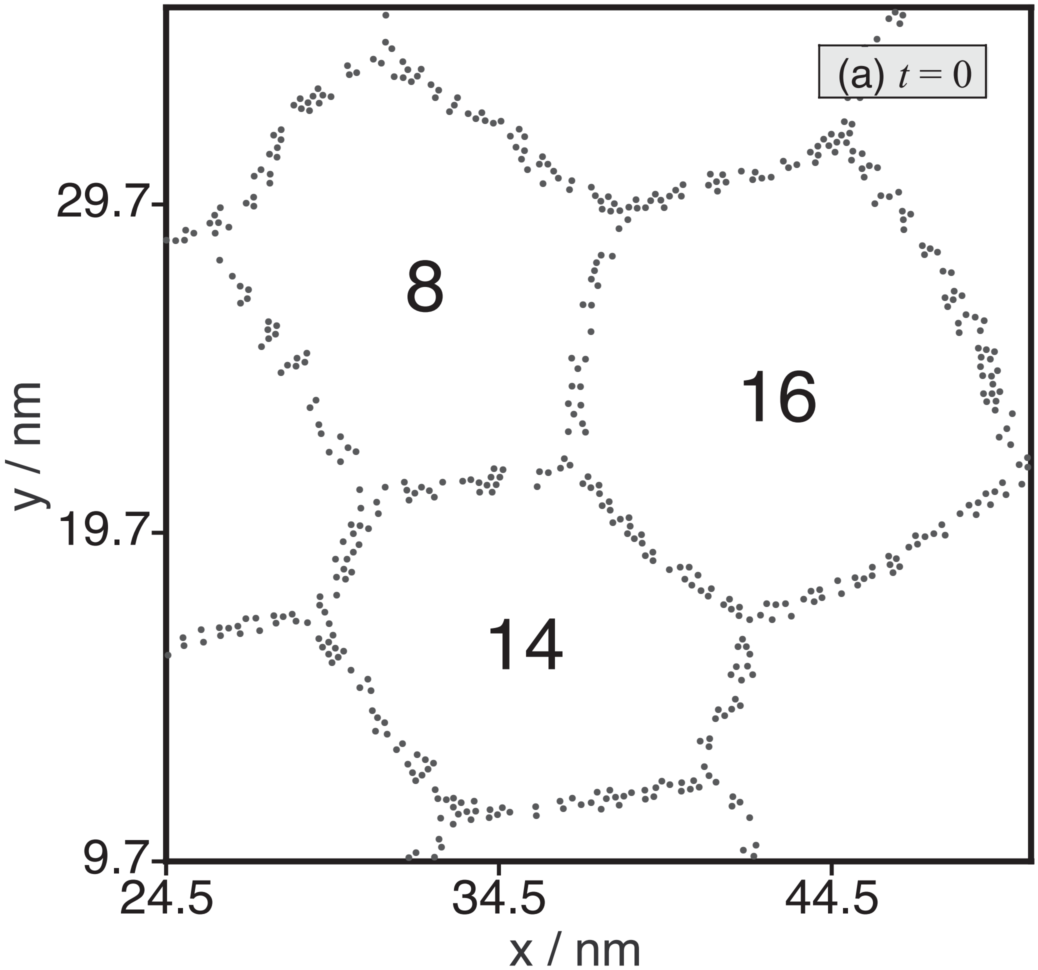
(e) t = 6.19ns
24
9
6
15
2
85
75
65
55
y / nm
30
40
50
60
x / nm

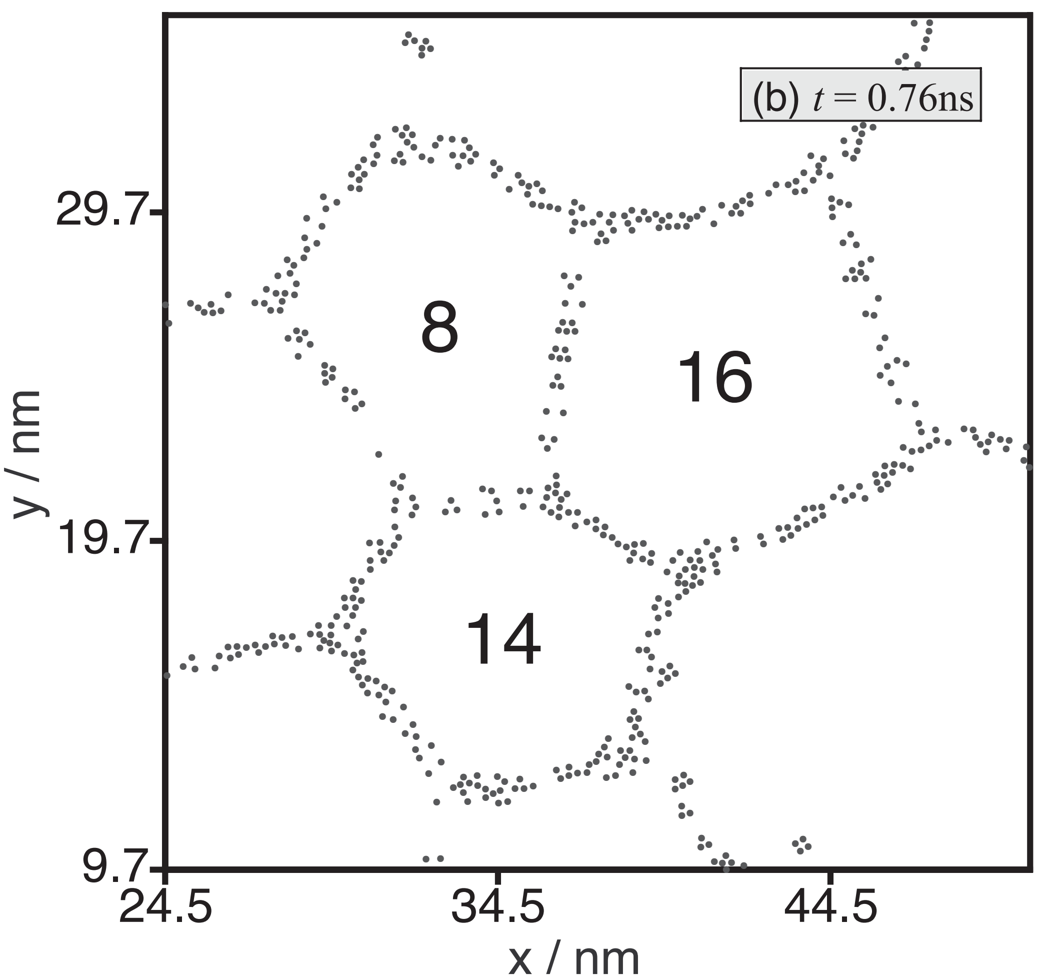
Grain-rotation-induced grain coalescence

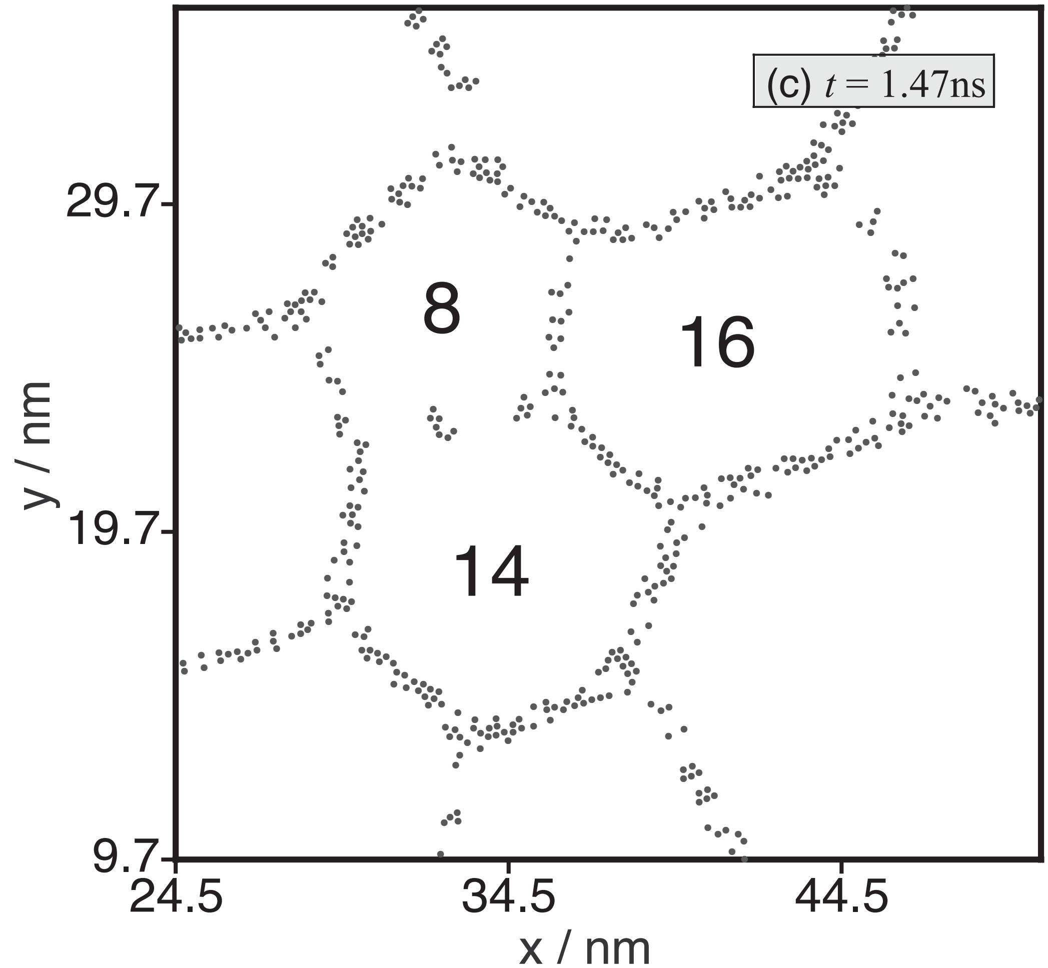
(A. Haslam et al., *Mat. Sci & Engin. A* 318, 293, 2001)

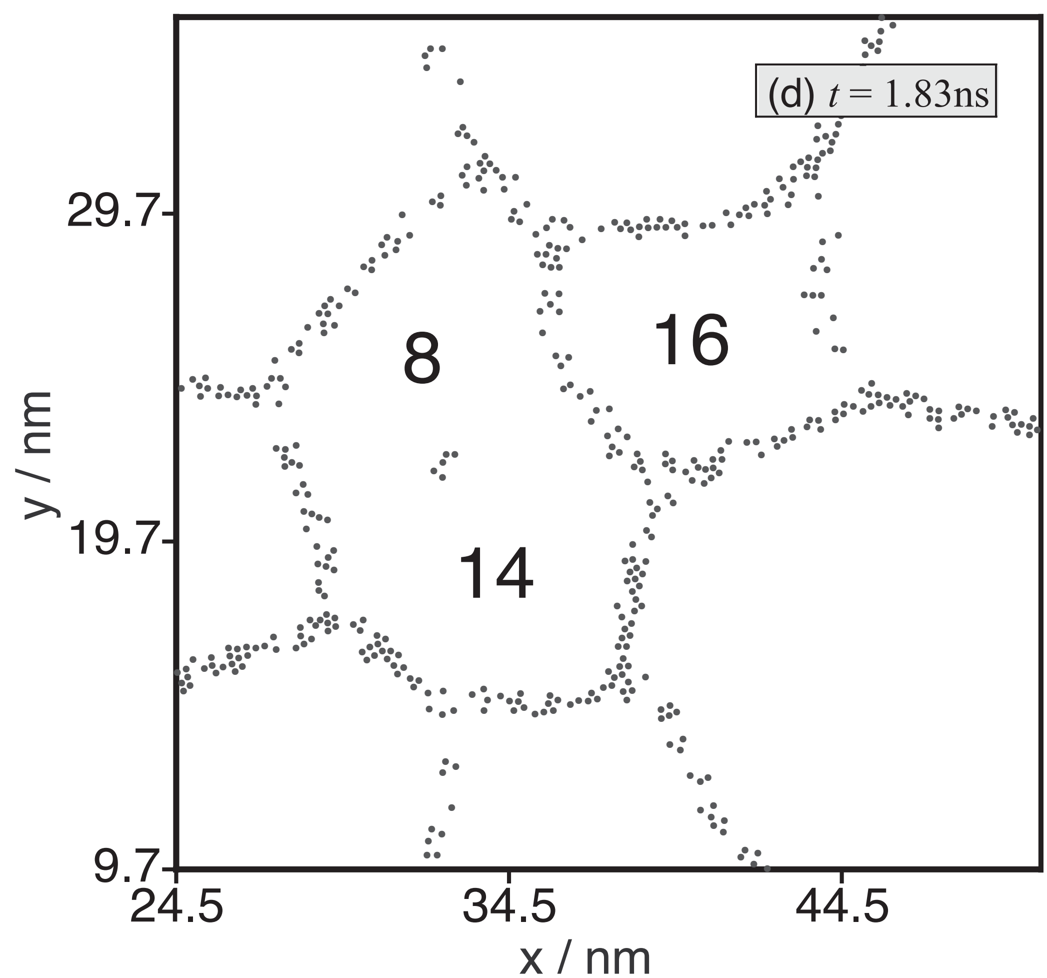


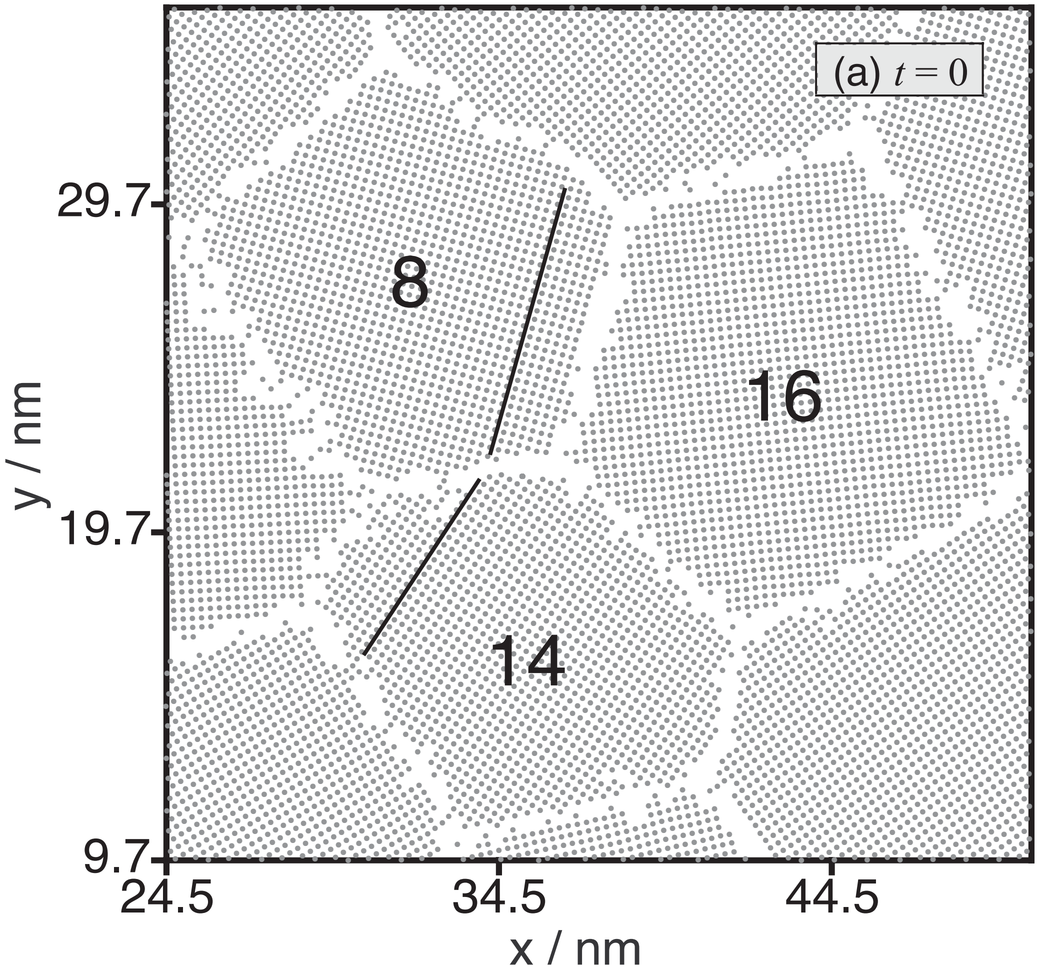



(a) $t = 0$
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm

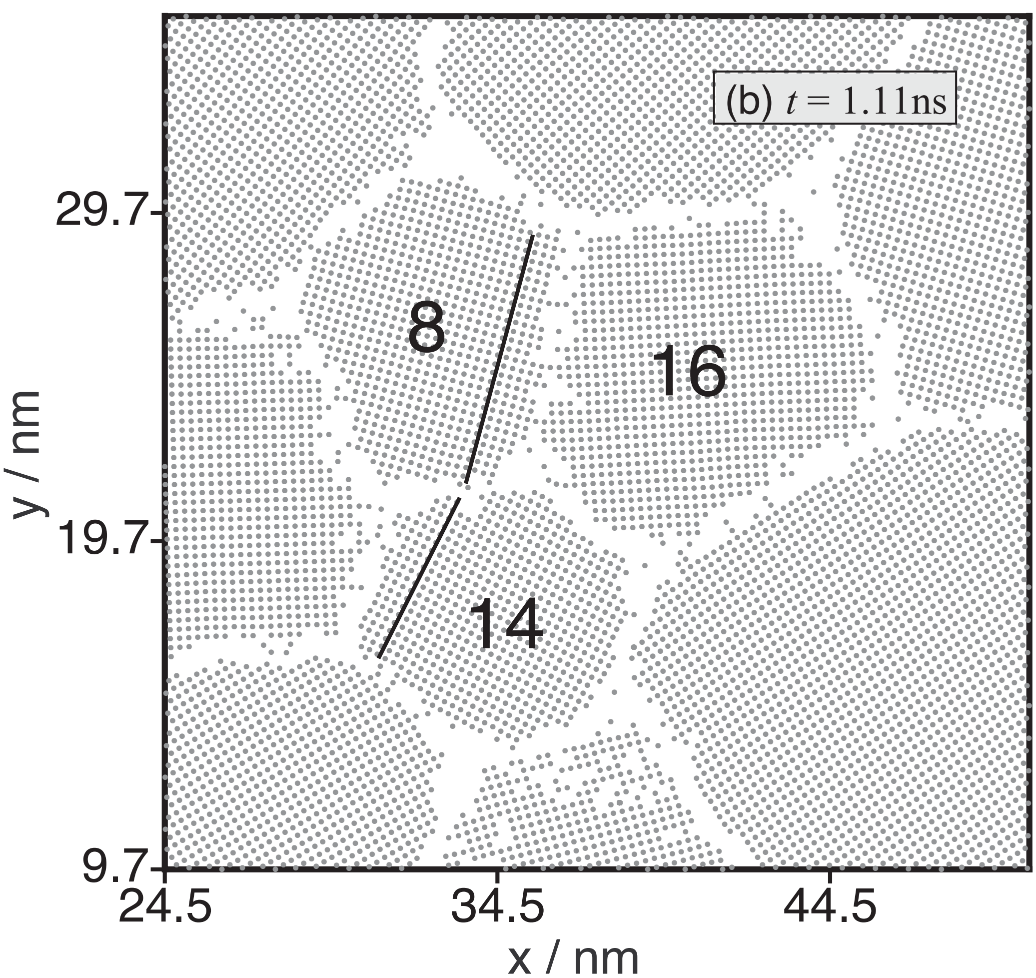

(b) $t = 0.76$ns
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm


(c) t = 1.47ns
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
x / nm
y / nm

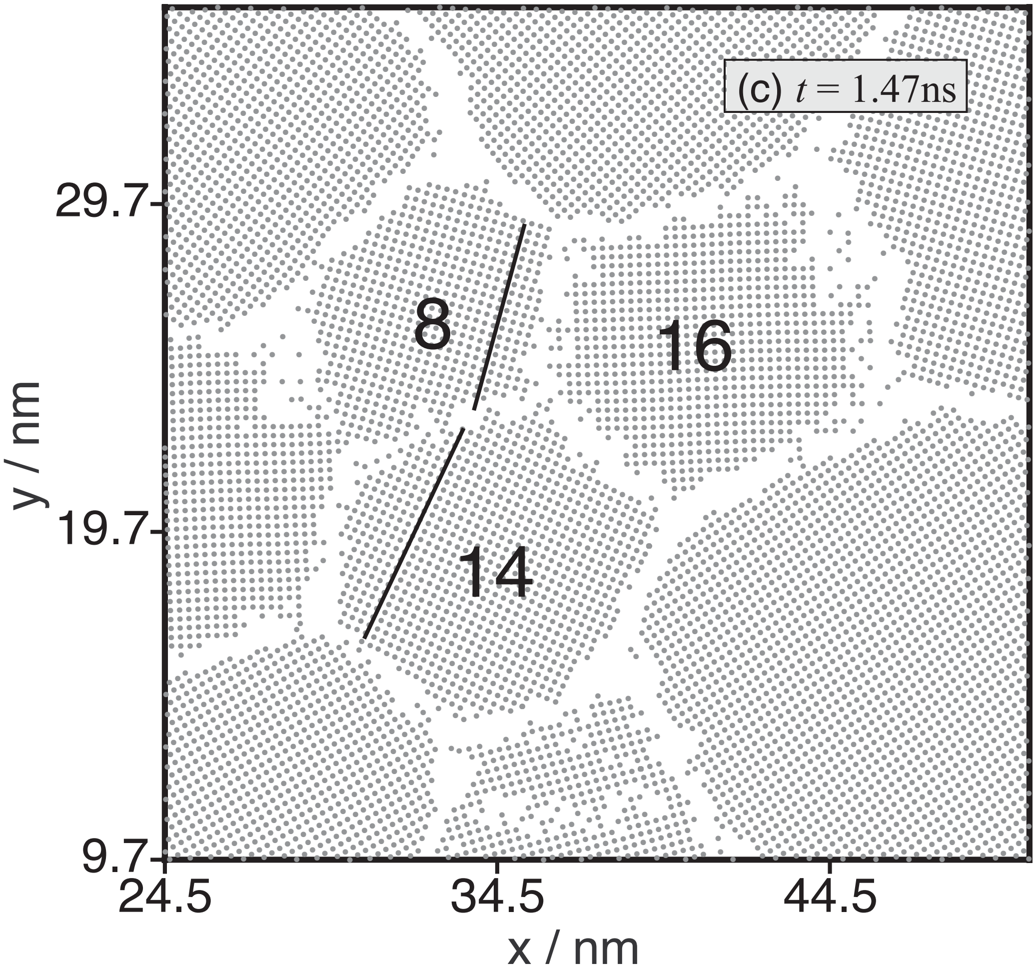

(d) t = 1.83ns
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
x / nm
y / nm



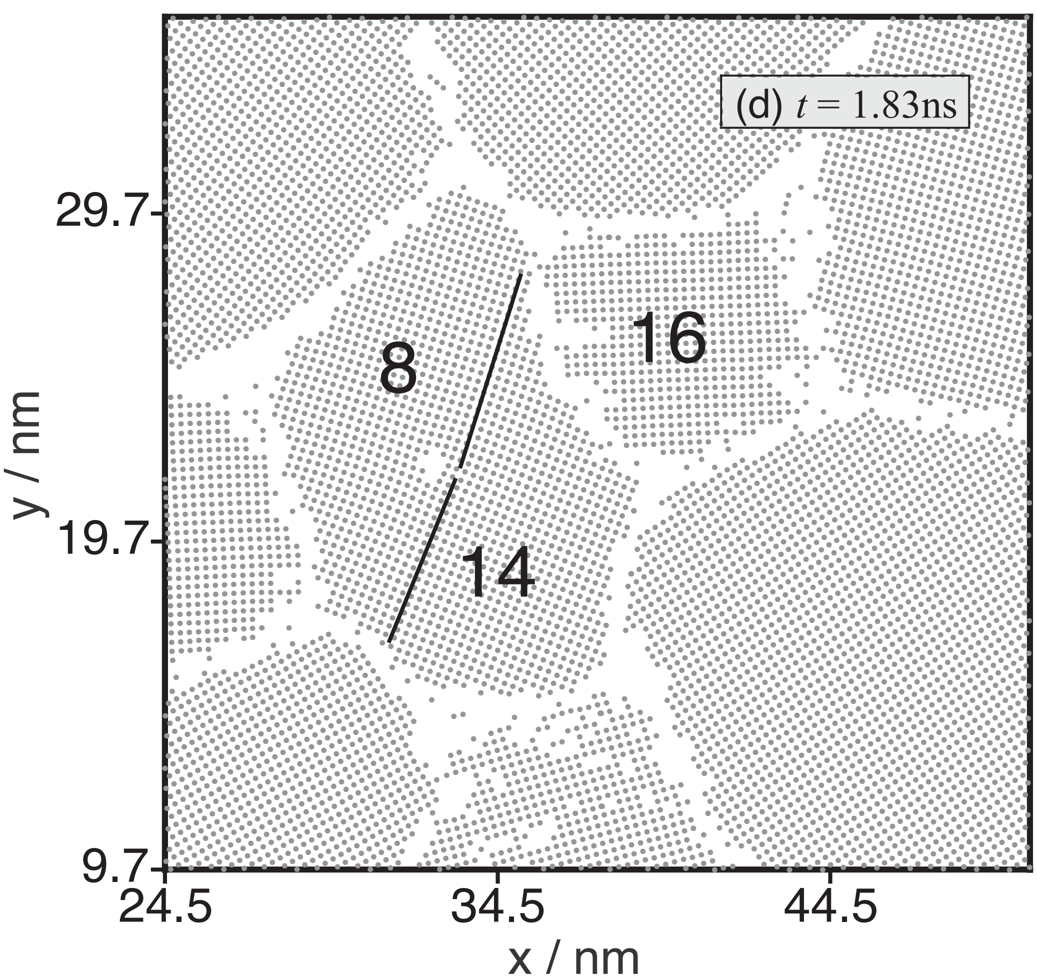
(a) $t = 0$
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm



(b) $t = 1.11$ns
8
16
14
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm

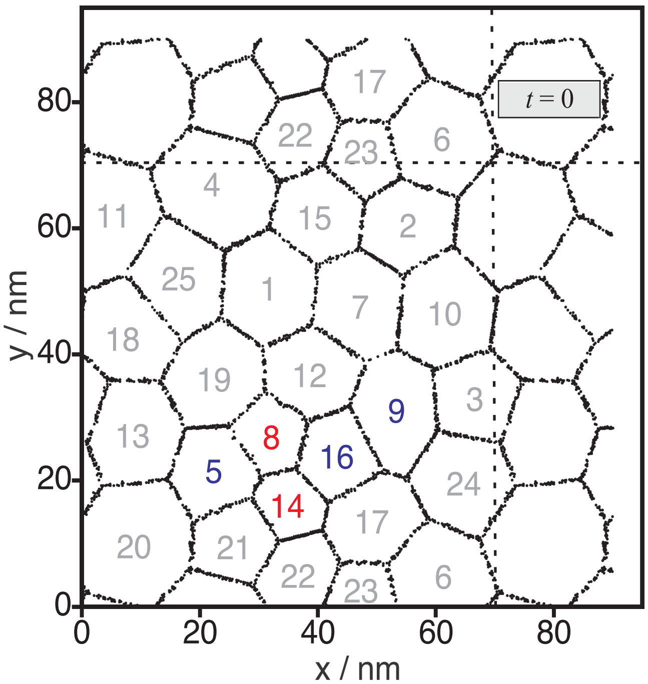


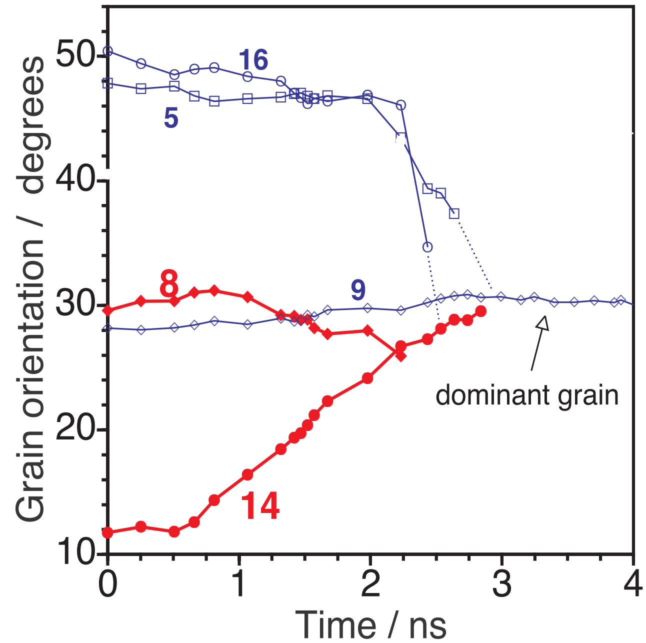
(c) t = 1.47ns
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm
8
16
14



(d) t = 1.83ns
29.7
19.7
9.7
24.5
34.5
44.5
y / nm
x / nm
8
16
14

Grain Rotation





OUTLINE

- *High-temperature deformation of nanocrystalline materials*
  - **High strain rates in MD simulations are meaningful**
  - **Unique capability of computer simulation to consider idealized microstructures**
  - **Enables deconvolution of the interplay between various processes**

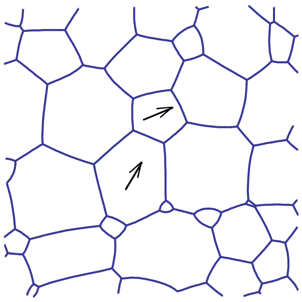
- *Atomic-level simulation of grain growth*
  - **Curvature-driven GB migration**
  - **Grain coalescence by coordinated grain rotations speeds up growth rate**
  - **Rotation rate ~ d^{-4}**

- *Mesoscale simulation of grain growth*
  - **Viscous law of motion for the grain boundaries and grains**
  - **Length scale given by grain size, time scale by GB mobility**
  - **Growth law, topology**

- *Ultimate goal: FEM simulations with microstructural materials input*

Theory of diffusion accommodated grain rotation

(D.Moldovan et. al., *Acta mater*. 49, 3521 (2001); based on Raj&Ashby, 1971)

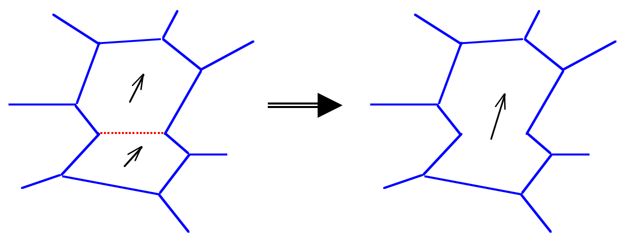


$$\tau = \sum_{k=1}^{Nsides} L_k \left(\frac{d\gamma}{d\theta}\right)_k$$ "cumulative torque"

$$\omega = M(R)\,\tau$$ viscous-like rotation

$$M(R) = \frac{A(\Omega, \delta D_{GB}, T, shape)}{R^5}$$ diffusion accommodated

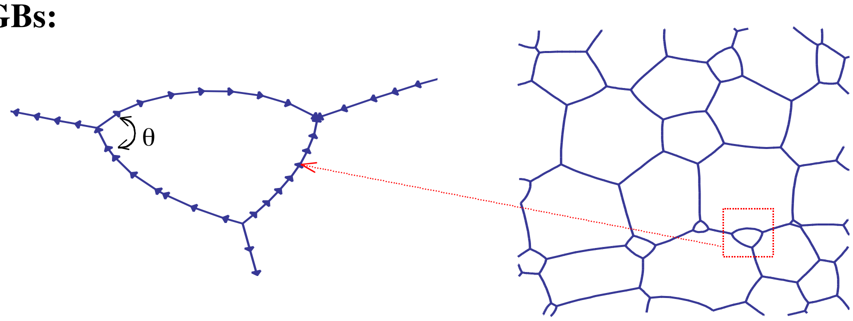
Grain coalescence by grain rotation



Mesoscale Simulations (2d)

(D.Moldovan et al., *Phil. Mag. A* 82, 1271, 2002)

- **Discretized GBs:**



- **Needleman-Rice (1980) variational functional for dissipated power (Cocks, 1992):**

$\Pi_m (v; k, \gamma, \mu)$ — GB velocity; Local GB curvature; GB energy; GB mobility

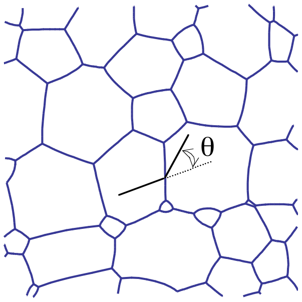
$\Pi_r (\omega; \tau_i , M_i)$ — Angular velocity; Torque; Rotational mobility

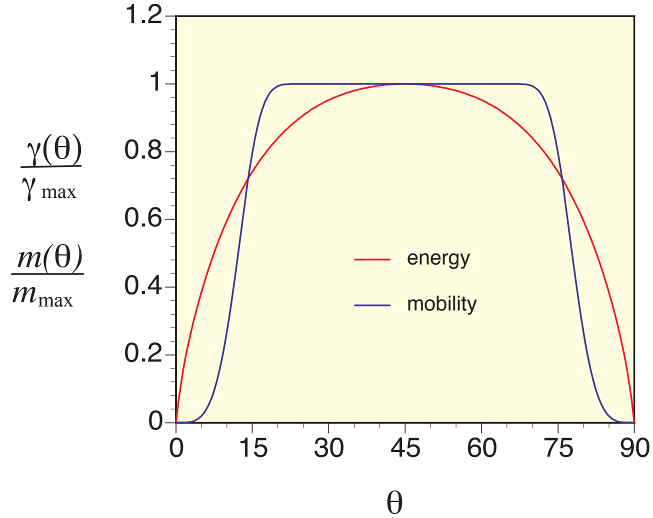
- **Viscous force laws** *(replaces Newton's law)*:

$v = \mu f$; $\omega_i = M_i \tau_i$; $M_i \sim d^{-5}$; $\omega_i \sim d^{-4}$; (D. Moldovan et al., *Acta mater*. 2001)

- **Velocity Monte-Carlo Simulation** (F. Cleri, *Physica*, 2000)
- **Triple-point equilibrium condition (Herring relation) not enforced *a priori*.**

Anisotropic grain-boundary properties ; <001> tilt boundaries





$$\frac{\gamma(\theta)}{\gamma_{\max}} = \sin(2\theta)\left[1 - \frac{E_s}{E_c}\ln(\sin(2\theta))\right]$$

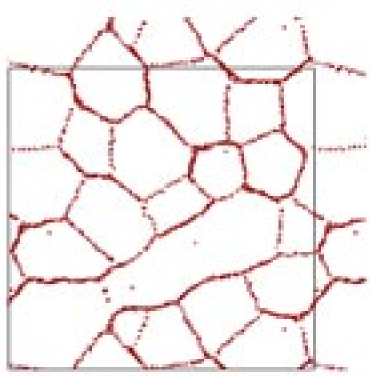
(Extended Read-Shockley)

$$\frac{m(\theta)}{m_{\max}} = 1 - \exp[-B(\frac{\theta}{\theta_0})^n]$$

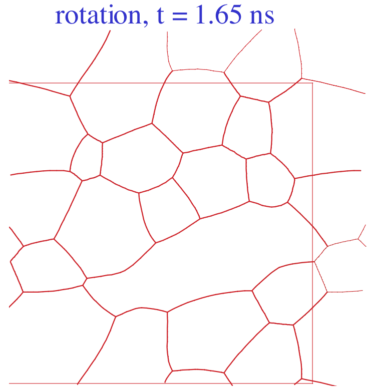
(Humphreys)

Validation of Mesoscale Simulation Methodoogy

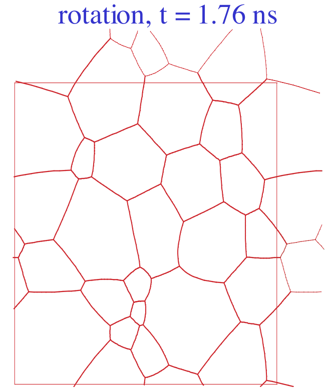
atomistic, t = 2.89 ns

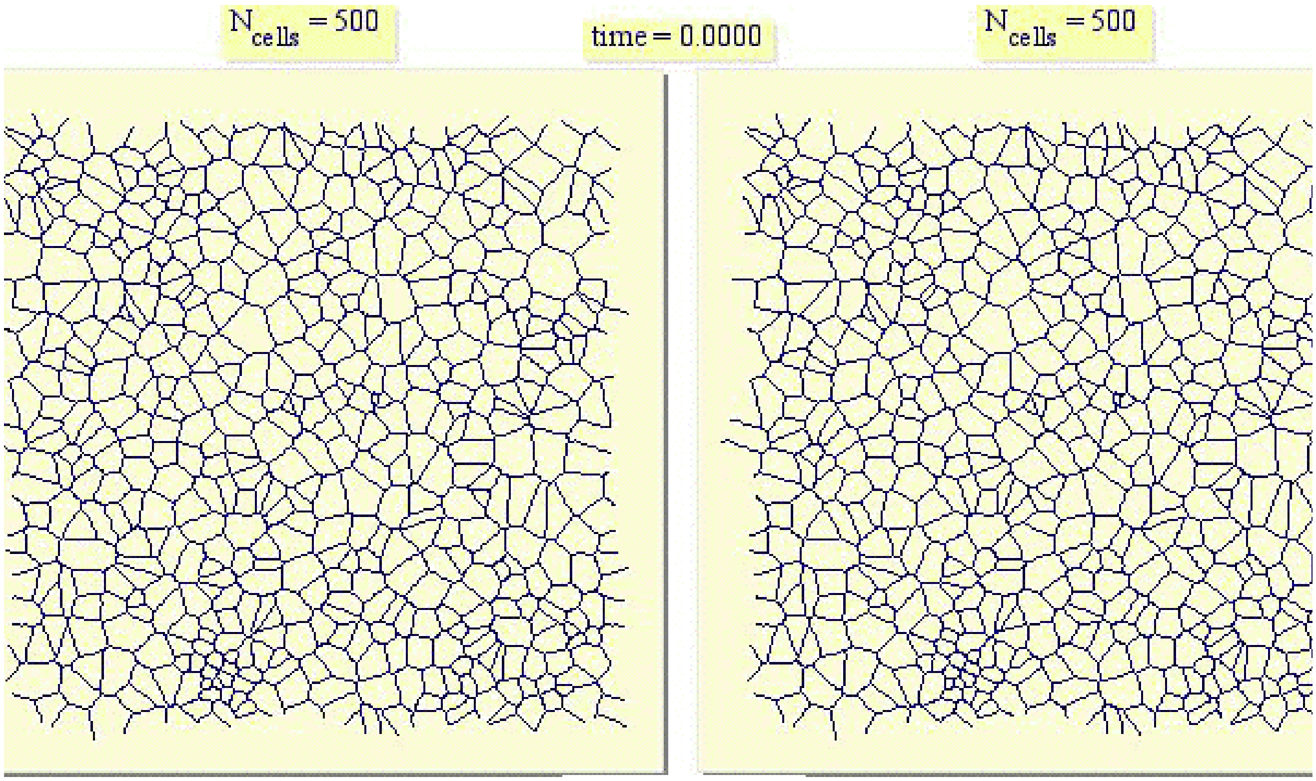


mesoscopic with grain rotation, t = 1.65 ns



mesoscopic without grain rotation, t = 1.76 ns

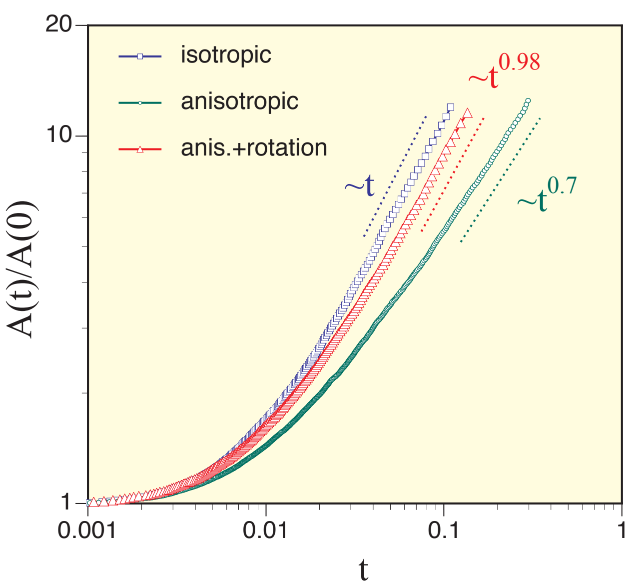




No grain rotation

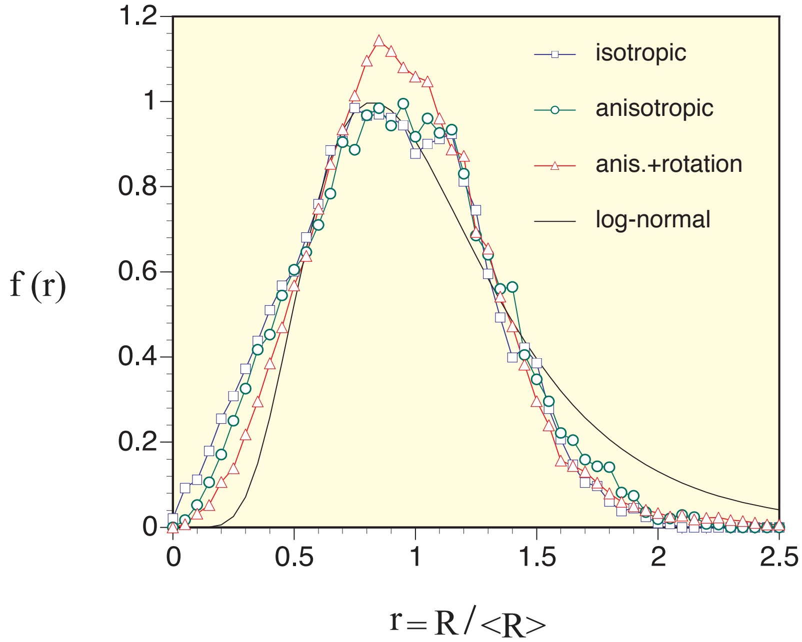
With grain rotation

Growth law



- Asymptotic power law at large times: $A(t) \sim t^{\alpha}$
  - isotropic $\alpha = 1.00 \pm 0.02$
  - anisotropic $\alpha = 0.70 \pm 0.02$
  - anisotropic+grain rotation: $\alpha = 0.98 \pm 0.02$

Grain size distribution function



- Rotation leads to a narrower grain-size distribution function

Grain growth as case study

- ***MD simulation***

  Identify growth mechanisms:
  - Curvature-driven GB migration
  - Grain-rotation-induced grain coalescence

- ***Mesoscale simulation***

  Capture MD results quantitatively
  Principle of virtual-power dissipation
  Incorporation of both growth mechanisms
  Modification of growth law and growth topology

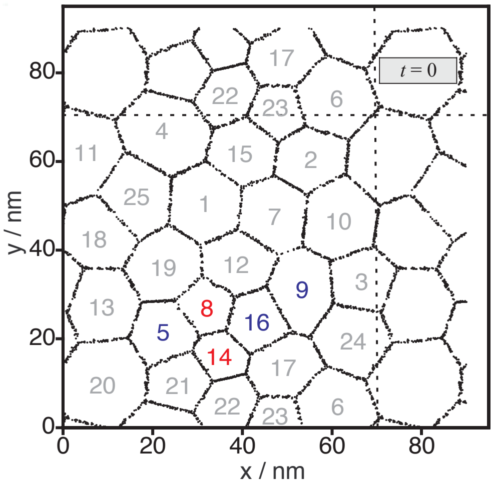
What is still missing are the effects of stress!

Interfacial Materials Group, Materials Science Division
Argonne National Laboratory

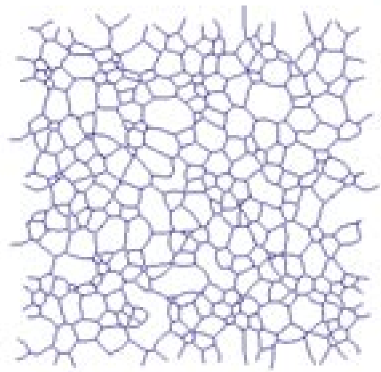
Multiscale Simulation of Microstructural Evolution @ANL

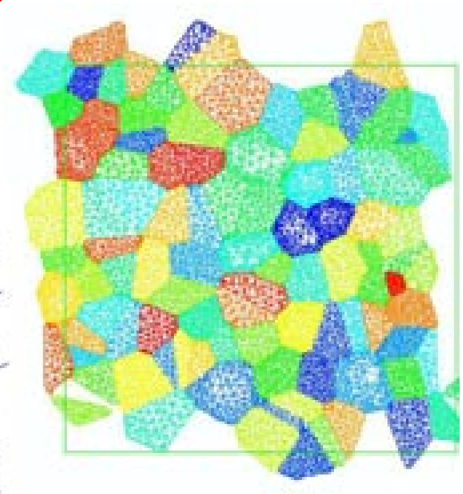
Atomistic

Finite element



Mesoscale





Newton's Law

Continuum level

Principle of virtual-power dissipation

Goal: Continuum simulations based on fundamental understanding of GB physic