The Potts Model
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References


Monte Carlo Method

Square 3D grid

1-6 : six 1st nearest neighbors
7-18 : twelve 2nd nearest neighbors
19-26 : eight 3rd nearest neighbors

System Energy:

\[ E = \frac{1}{2} \sum_{j} \sum_{i} \{ \gamma(S_i, S_j)(1 - \delta_{S_i S_j}) + F(S_j) \} \]

Total number of spins/grains

Number of nearest neighbors

Grain Boundary Energy

Stored Energy

Reorientation Probability:

\[ P = \begin{cases} 
\frac{\gamma(S_i, S_j) \mu(S_i, S_j)}{\gamma_{\text{max}} \mu_{\text{max.}}} \times 1 & \Delta E \leq 0 \\
\frac{\gamma_{\text{max}} \mu_{\text{max.}}}{\gamma(S_i, S_j) \mu(S_i, S_j)} \times \exp \left( -\frac{\Delta E}{T} \right) & \Delta E > 0 
\end{cases} \]
Potts model

\[ E = \sum_{i} \sum_{j} J(S_i, S_j) \left( 1 - \delta_{S_i S_j} \right) \]

\[ P = \begin{cases} 
\frac{J(S_i, S_j) \mu(S_i, S_j)}{J_{\text{max}} \mu_{\text{max}}} \times 1 & \Delta E \leq 0 \\
\frac{J(S_i, S_j) \mu(S_i, S_j)}{J_{\text{max}} \mu_{\text{max}}} \times \exp\left(\frac{-\Delta E}{T}\right) & \Delta E > 0 
\end{cases} \]

- \( E \): system energy
- \( P \): transition probability
- \( J \): interaction energy
- \( \mu \): mobility
- \( S \): orientation

2 unlike nearest neighbors
6 unlike next nearest neighbors
Modification for variable lattice $T$

- Large (>2) variation in grain boundary energy with finite lattice temperature can lead to excessive roughness of a low energy boundary.
- Variable lattice temperature used to ensure uniform roughness on all boundaries because a large range in g.b. energy required (Read-Shockley, e.g.).
- Abnormal grain growth investigations have also suggested scaling the lattice temperature based on the local grain boundary energy (all in 2D).
- This has been found to allow the model to correctly match the expected variation in shrinkage rates of isolated (circular) grains, and to match the predicted abnormal growth of polycrystalline structures (Radhakrishnan).
**MC method: temperature scaling**

Conventional: \( P(S_i, S_j, \Delta E, T) = \begin{cases} \frac{J(S_i, S_j)}{J_{\text{max}}} \frac{M(S_i, S_j)}{M_{\text{max}}} & \Delta E \leq 0 \\ \frac{J(S_i, S_j)}{J_{\text{max}}} \frac{M(S_i, S_j)}{M_{\text{max}}} \exp(-\Delta E/kT) & \Delta E > 0 \end{cases} \)

Temperature Scaling: \( P(S_i, S_j, \Delta E, T) = \begin{cases} \frac{J(S_i, S_j)}{J_{\text{max}}} \frac{M(S_i, S_j)}{M_{\text{max}}} & \Delta E \leq 0 \\ \frac{J(S_i, S_j)}{J_{\text{max}}} \frac{M(S_i, S_j)}{M_{\text{max}}} \exp \left( -\frac{\Delta E}{kT(J(S_i, S_j))} \right) & \Delta E > 0 \end{cases} \)
Test: columnar growth

Fixed Temperature

Temperature $\propto \gamma$
Temperature scaling: shrinking circle results

Lattice: square, with 1st and 2nd nearest neighbors (wild flips allowed)
Parallel Monte Carlo Algorithm

The algorithm is a modification of the original Ising model.

- **System Energy** ($E$): $E = \frac{1}{2} \sum_1^N \sum_{i=1}^z J(S_i, S_j) \left( -\delta_{S_i, S_j} \right)$

- **Spin-flip probability** ($p$):
  - $\Delta E \leq 0$  \quad \quad \quad p(\Delta E) = M(S_i, S_j) \times J(S_i, S_j)$
  - $\Delta E > 0$  \quad \quad \quad p(\Delta E) = M(S_i, S_j) \times J(S_i, S_j) \times \exp \left[ -\frac{\Delta E}{J(S_i, S_j)T} \right]

- **Single Processor sweep sequence:**
  1. Pick a site at random
  2. Pick a new spin value from one of its neighbors
  3. Calculate $\Delta E$
  4. Accept or reject change based on $p(\Delta E)$

$J(S_i, S_j) = \text{GB Energy}$
$M(S_i, S_j) = \text{Mobility}$
$E = \text{Energy}$
$T = \text{Temperature (artificial)}$
$nn = \text{nearest neighbors}$
$N = \text{Total lattice sites}$
$\delta = \text{Kronecker Delta}$
$S_i = \text{Spin Value}$
Parallel Monte Carlo Algorithm

- Division of microstructure into subdomains
  - Boundary Sites? Use GHOST CELLS
  - Illegal Flips? Apply checkerboard masks
  - Synchronous? Update processors at common points

- Multi-processor Sweep Sequence:

  Start Color Loop(B, HS, DS, W)
  
  Loop over lattice sites of color I
  
  1.  
  a. Pick a site at random
  b. Pick new spin value
  c. Calculate $\Delta E$
  d. Accept or reject change

  2. Exchange boundary information with neighbor processors

  End lattice site loop

  End Color Loop

S.A. Wright et al., Sandia Report#SAND97-1925.
Inter-processor Communication

How do processors send information?

1. Call to MPI library function returns information about 6 neighbors =
   (North, South, East, West, Up, Down)

2. Information can be sent to neighbor by specifying destination as (nodenorth, nodesouth, nodeeast, nodewest, nodeup, nodedown)
Inter-processor Communication

Processor A sends its boundary sites to the right (processor B).
Information stored in “ghost cells” of $B[i=0,j]$

Reversal: B sends its boundary sites to the left (processor A).
Information is stored in “ghost cells of $A[imax+1,j]$"
**Model Validation**

**Objective:** To determine whether this PMC algorithm can reproduce curvature-driven grain growth.

\[ \vec{v} = M \gamma \frac{2}{R} \]

Linear relationship exists between area and time.
Model Validation

PARAMETERS:
200$^3$ box
T=1.7
Initial Radius = 50
Isotropic Grain Boundary Properties

Results confirm the sphere is shrinking in an isotropic manner towards its center of curvature.

Parallel MC algorithm obeys conditions for curvature-driven grain growth; PMC will be used to simulate grain growth.
Efficiency and Scalability

**Objective:** To determine the scalability and efficiency of a synchronous parallel Monte Carlo algorithm as a function of the number of processors and processor workload on a supercomputing and beowulf network.

Nomenclature:

```
msca01
```

- **Machine:**
  - m=mrsec
  - l=lemieux
  - r=roberts

- **Style:**
  - eff=efficiency
  - sca=scalability

- **Run #:**

Variables:

1. # Processors
2. Workload
3. Hardware
Scalability

Maintain a constant subdomain size as more processors are added.

Total time

Subtracted I/O time

I/O Operation:
Each slave node sends array information to master node.
Master node writes to file.
Efficiency

• Maintain a constant TOTAL domain while increasing the number of processors.

Q: If a man can dig a hole in 60 minutes, can 60 men dig a hole in 1 minute?

Physical limitations exist which remove this curve from a linear relationship. Most common culprit is “interprocessor communication”!!

For our experiment, a near-linear relationship exists up to 256 processors.
Memory Performance

• Cache Performance

• Cache Definition: A memory area where frequently accessed data can be stored for rapid access

  1.7% Miss rate determined for PMC code

  PSC Standard lists >10% as poor Cache usage

• MFLOPs Performance

• MFLOPs Definition: MFLOPS is an abbreviation of floating point operations per second. This is used as a measure of a computer's performance, especially in fields of scientific calculations that make heavy use of floating point calculations.
Grain Growth Study

**Objective:** Determine kinetic behavior for isotropic and anisotropic grain boundary properties.

1. Self Similarity – structure looks identical to previous state if examined at a different magnification.

2. Grain Growth Kinetics

   \[ \vec{v} = M \gamma \kappa \]

   \[ A - A_0 = K t^n \]

   Theoretical calculations yield \(n = 1\). Values close to 1 have been found for very pure metals annealed close to their melting points.

3. Unimodal Grain Size Distributions

Grain Growth Study

- Evolution of microstructure using isotropic GB properties


**Texture Description**

- Monte Carlo Model works with a set of discrete orientations
  - Conventional: scalar parameter, \( S \in (1..Q) \), spin number
  - Texture: assign (3-parameter) orientation, \( g_i(\Psi, \Theta, \phi) \) to each spin number, \( S_i \): \( \Psi, \phi \in (0..2\pi) \), \( \Theta \in (0..\pi/2) \)
- Calculate the disorientation for each combination of grains and associated properties.
- Make a look-up table of all required properties before starting evolution simulation.

\[
\begin{array}{|c|c|c|c|}
\hline
 & S_1 (\Psi_1, \Theta_1, \phi_1) & S_2 (\Psi_2, \Theta_2, \phi_2) & \ldots & S_n (\Psi_n, \Theta_n, \phi_n) \\
\hline
S_1 & - & \Delta g_{12} & & \Delta g_{1n} \\
\hline
S_2 & & - & & \Delta g_{2n} \\
\hline
\vdots & \vdots & \vdots & \ddots & \vdots \\
\hline
S_n & & & & - \\
\hline
\end{array}
\]
**Simulation: kinetic Monte Carlo**

- Triangular 200 x 200 grid, 1st & 2nd nearest neighbors, Q=500, spin no. linked to orientation.
- Equiaxed initial grain structure with ~4000 grains.
- G.B. properties for unalloyed Al, as measured.

\[
S_1(\Psi_1, \Theta_1, \phi_1) \quad S_2(\Psi_2, \Theta_2, \phi_2) \quad \cdots \quad S_n(\Psi_n, \Theta_n, \phi_n)
\]

<table>
<thead>
<tr>
<th>( S_1 )</th>
<th>( S_2 )</th>
<th>( \cdots )</th>
<th>( S_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-</td>
<td>( \gamma(\Delta g_{12}) ), ( M(\Delta g_{12}) )</td>
<td>( \gamma(\Delta g_{1n}) ), ( M(\Delta g_{1n}) )</td>
<td></td>
</tr>
<tr>
<td>( S_2 )</td>
<td>-</td>
<td>( \gamma(\Delta g_{2n}) ), ( M(\Delta g_{2n}) )</td>
<td></td>
</tr>
<tr>
<td>( \vdots )</td>
<td>( \vdots )</td>
<td>( \gamma(\Delta g_{2n}) ), ( M(\Delta g_{2n}) )</td>
<td></td>
</tr>
<tr>
<td>( S_n )</td>
<td>( \gamma(\Delta g_{2n}) ), ( M(\Delta g_{2n}) )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
M = M_0 \left( 1 - 0.99 e^{-0.5 \theta^9} \right)
\]
Grain Growth Study

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$R_0$</th>
<th>$T$</th>
<th>$n$</th>
</tr>
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<tbody>
<tr>
<td>nggl01</td>
<td>7.32</td>
<td>1.5</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl02</td>
<td>7.32</td>
<td>1.0</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl03</td>
<td>7.32</td>
<td>1.5</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl04</td>
<td>7.32</td>
<td>1.5</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl05</td>
<td>7.32</td>
<td>1.5</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl06</td>
<td>1.50</td>
<td>1.5</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl07</td>
<td>1.50</td>
<td>0.0</td>
<td>1.20</td>
</tr>
<tr>
<td>nggl08</td>
<td>1.50</td>
<td>0.1</td>
<td>1.20</td>
</tr>
<tr>
<td>aniso6</td>
<td>1.50</td>
<td>1.5</td>
<td>0.99</td>
</tr>
<tr>
<td>aniso7</td>
<td>1.50</td>
<td>0.0</td>
<td>0.86</td>
</tr>
<tr>
<td>aniso8</td>
<td>1.50</td>
<td>1.5</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Exponent value indicates microstructure is coarsening too fast.

Source of problem??

MC is a stochastic model, which implies random events must occur. By selecting the checkerboard randomly, the exponent has been reduced by $\sim 0.25$!!!
Grain Growth Study UPDATE

- Evolution of microstructure using isotropic GB properties
- Closer agreement with the ideal case. The change in area should be linearly proportional to time ($n=1.0$)

$$A - A_0 = K t^n$$
Model Validation

200³ box
T=1.5
Isotropic Grain Boundary Properties

Results confirm the sphere is shrinking in an isotropic manner
Temperature parameter should be equal to or greater than 1.5
Model Validation

Objective: To determine whether this PMC algorithm can reproduce curvature-driven grain growth.

\[ \mathbf{v} = \mathcal{M} \gamma \frac{2}{R} \]

Linear relationship exists between area and time.
Grain Growth Study

- Grain Size Distribution is invariant with time

Peak fluctuations occur at late times when $N_G$ is small.
N-fold way model

• Concepts
  - Poisson Processes
  - Continuous time

• Monte Carlo Simulation Algorithms
  – Metropolis (conventional)
  – N-fold Way

• Connection between Poisson Process and “N-fold way” model

• Summary
Poisson Processes

• A Poisson process is a stochastic process which is defined in terms of the occurrences of events. Also, the number of events between time $a$ and time $b$ is given as $N(b) - N(a)$ and has a Poisson distribution.

• The probability that there are exactly $k$ occurrences during unit time ($k$ being a non-negative integer, $k = 0, 1, 2, ...$) is

$$f(k; \lambda) = \frac{e^{-\lambda} \lambda^k}{k!},$$

Where
- $e$ is the base of the natural logarithm ($e = 2.71828...$)
- $k$ is the number of occurrences of an event
- $k!$ is the factorial of $k$
- $\lambda$ is a positive real number, equal to the expected number of occurrences that occur during the given interval.

Note: This probability distribution may be deduced to

$$\Pr(T > t) = \Pr(N_t = 0) = e^{-\lambda t}.$$
Examples of Poisson Processes

• The number of telephone calls arriving at a switchboard per hour.
• The number of webpage requests on a server, except for denial of service attacks.
• The number of photons hitting a photodetector, when lit by a laser source.
• The number of particles emitted via radioactive decay by an unstable substance.
• Spin flippings in Monte Carlo n-fold way model (our focus)
General characteristics of a Poisson process

There are only two conditions for a stochastic process to be a Poisson process.

1. **Orderliness:**

\[ \lim_{\Delta t \to 0} P(N(t + \Delta t) - N(t) > 1 \mid N(t + \Delta t) - N(t) \geq 1) = 0 \]

Arrivals don’t occur simultaneously.

2. **Memorylessness:**

The number of arrivals occurring in any bounded interval of time \( t \) is independent of the number of arrivals occurring before time \( t \).
In probability theory, a **continuous-time Markov process** is a stochastic process \( \{ X(t) : t \geq 0 \} \) that satisfies the **Markov property** and takes values from a set called the **state space**.

The **Markov property** states that at any time \( s > t > 0 \), the conditional **probability distribution** of the process at time \( s \) given the whole history of the process up to and including time \( t \), depends only on the state of the process at time \( t \).
Monte Carlo Simulation
-- Metropolis Algorithm

The key steps of this algorithm are as given below (Landau and Binder 2000):

1. Choose a site $i$ at random
2. Calculate the energy change associated with changing the spin at the $ith$ site
3. Generate a random number $r$ such that $0 < r < 1$
4. If $r < \exp(-\Delta E/k_B T)$, flip the spin
5. Increment time regardless of whether a site changes its spin or not
6. Go to 1 until sufficient data is gathered.

Disadvantages:
- During the late stages of evolution the transition probability approaches 0 at most sites.
- For low temperatures, flipping probability is low.
Steps of n-fold way algorithm

1. Generate a random number $r \in (0,1]$.
2. Choose a class $k$ that satisfies the condition given in Equation
   $$Q_{k-1} \leq rQ_n < Q_k.$$
3. Generate a random number to choose one of the sites from class $k$.
4. Flip the spin at the chosen site with probability 1.
5. Update the class of the chosen spin and all of its nearest neighbors
   $$Q_n = \sum_{j=1}^{n} n_j p_j.$$
6. Determine activity $Q_n$.
7. Go to 1 until sufficient data is gathered.

Advantage: Eliminate the need to unsuccessful changes by calculating the spin-flip transition probability for each of the lattice sites before choosing a site to flip for a given state of the system.
A specific case of Poisson Process

A Poisson process is characterized by a rate parameter $\lambda$, also known as intensity.

$$\Pr(T > t) = \Pr(N_t = 0) = e^{-\lambda t}.$$  \hspace{1cm}  $$\Pr(T > t) = P(N_t \geq 1) = 1 - e^{-\lambda t}$$

Probability of occurrence vs. time.
**Derivation of Time increment (Link)**

In the n-fold way, every spin flip attempt is successful, so the n-fold way time increment must be scaled by the average time between successful flips in the conventional Monte Carlo scheme.

\[ \tau = 1MCS \quad A = \sum_{i=1}^{N} \sum_{j=1}^{Q-1} p_{ij}(S_i - S_j) \quad \langle \tau \rangle = \frac{A}{N(Q-1)} \quad \dot{\tau} = \frac{N \langle \tau \rangle}{(Q-1)\tau} = \frac{A}{(Q-1)\tau} \]

Probability that no successful flip has occurred in the time interval \( \Delta t \)

\( g(\Delta t) \)

Probability that no successful flip has occurred in the time interval \( \Delta t + dt \)

\( g(\Delta t + dt) \)

\[ g(\Delta t + dt) = g(\Delta t) \cdot g(dt) \]

\[ g(dt) = 1 - \dot{\tau} dt = 1 - \left( \frac{A}{(Q-1)\tau} \right) dt \]

\[ g(\Delta t + dt) = g(\Delta t) \cdot \left( 1 - \frac{A}{(Q-1)\tau} dt \right) = g(\Delta t) + \frac{dg(\Delta t)}{dt} dt \]

\[ \frac{dg(\Delta t)}{g(\Delta t)} = -\frac{A}{(Q-1)\tau} dt \quad \ln[g(\Delta t)] = -(A/\tau(Q-1))\Delta t \]

Poisson distribution!

\[ \Delta t = -\left( \frac{(Q-1)\tau}{A} \right) \ln R \]
Summary

• Monte Carlo n fold way algorithm can be effectively treated as a Poisson process.
• Continuous time is applied in Monte Carlo simulation.
• Monte Carlo n-fold way algorithm is more efficient for relatively high temperatures or in larger data sets than conventional models.
An example of classes  (Ising Model)

Figure 4.2: Three examples of different classes in the n-fold way algorithm for a two-dimensional, square lattice Ising model. Each class represents a different possibility for a change in configuration of spins (or orientations when grain growth is considered). The spins are shown in their initial configuration and the transition probability is evaluated for changing (flipping) the central spin (from up to down).
Link “n-fold way” to Poisson Process

In effect, the time increment, $\Delta t$, in the n-fold way algorithm is correlated to the probability that the given system configuration will change to a different configuration during the time increment:

$$\Delta t = \frac{-(Q - 1)}{A} \ln r.$$  

$$A = \sum_{i=1}^{N} \sum_{j=1}^{Q-1} p_{ij} (S_i \rightarrow S'_j)$$

This equation is based on the assumption that the successful re-orientation of a site is described by an exponential probability distribution.

$$\Pr(T > t) = P(Nt \geq 1) = 1 - e^{-\lambda t}$$

Hence, successive evolution steps are Poisson events.
Simulation Approach

- 2D Monte Carlo model for grain growth: 200x200 triangular lattice; Q=500; lattice temperature = 0.35, scaled by energy for constant boundary roughness; 2000 grains coarsen to ~200 grains; 3D orientations.
- 3D Monte Carlo model: 100x100x100 domain with a (1,2,3) neighbor simple cubic lattice, temperature = 0.9 (some at 0.5; little sensitivity to lattice temperature); 10,000 grains at t=0.
- Texture mapped to a list of 500 discrete orientations; fcc rolling texture with ~6% near-cube grains added.
- Anisotropic grain boundary properties incorporated to modify the energy and mobility; values taken from experiment (low angle boundaries) and simulation (molecular dynamics by Upmanyu, Srolovitz at Princeton).
- Simulated annealing used to optimize placement of cube grains.
Grain Size Control

- Upper right panel illustrates the physics of boundary-particle interaction: $D_{\text{pinned}} \sim d_{\text{ppt}}/V_f$
- Lower right panel shows summary of experimental data, together with only available parallel calculations with Monte Carlo in 3D.
- Investigating the significant range of particle volume fraction drives us into the petascale; linear sizes of the required mesh indicated on graph.
- Monte Carlo method (Potts) offers only practical algorithm.

- CMU parallel results: Roberts
- Previous parallel results: Radhakrishnan
- Previous parallel results: Miodonwik

Experimental review: Manohar et al. 1998
Particle Induced Abnormal Grain Growth

The objective of the research was to examine the affect of non-random particle placement on the kinetics and limiting grain size. During the course of the investigation, abnormal grain growth (AGG) was observed in a few of the microstructures.

Microstructures were generated with an equiaxed morphology and a narrow grain size distribution (i.e. $R_{\text{max}}$ did not exceed $2.5 < R$). In a subsequent step, the microstructures were injected with inert, mono-sized particles. The particles were not randomly inserted, but preferentially placed on grain boundaries in specific fractions.

The simulations were conducted using a parallel version of the Potts-based Monte Carlo algorithm. Digital microstructures were $400^3$ voxels in volume and isotropic grain boundary properties were applied ($\gamma=1$, $M=1$).
List of configurations examined in the research project.

<table>
<thead>
<tr>
<th>Grain Size</th>
<th>Volume Fraction</th>
<th>Particle Fraction on Boundaries</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.6</td>
<td>0.04</td>
<td>0.30</td>
</tr>
<tr>
<td>11.7</td>
<td>0.06</td>
<td>0.50</td>
</tr>
<tr>
<td>15.2</td>
<td>0.08</td>
<td>0.70</td>
</tr>
<tr>
<td>18.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Ex: 0.04VV and 0.03 fraction on grain boundaries.

With 0.04V V of cubic particles (volume=27 voxels), the microstructure contains approximately 95,000 particles. Of these 95,000 particles, 30% or 28,500 will be situated on the grain boundaries and the remaining 70% will be located in the grain interiors.
Two-dimensional cross-section taken from the center of the modeling domain. An example of NGG and AGG is provided.

$R_0=18.4, 0.06V_V$, and 30% of particles on grain boundaries

$R_0=7.6, 0.04V_V$, and 70% of particles on grain boundaries
In the simulations with NGG, the pinned grain size is well below the Zener threshold; on the other hand, the AGG case does not have a limiting size.

The average growth rate does not behave in a similar fashion to other simulations exhibiting only NGG and boundary pinning.
In the abnormal case, the GSD appears to be uni-modal, but a secondary peak becomes apparent at late times.
Summary

Abnormal grain growth is observed in a particle-containing microstructure.

Isotropic grain boundary properties eliminate texture as a possible source for AGG.

AGG appears to be caused by a combination of grain size and local particle density fluctuations on grain boundaries.
4: Critical dispersion in orientation

- Abnormal grain growth is significant in the early stages of recrystallization of metals: coarsening of subgrain structures can generate nucleation.
- For coarsening within a single orientation (i.e. a subgrain structure) there appears to be a critical dispersion (spread) in texture.
  - Narrower dispersions lead to regular (self-similar) coarsening.
  - Larger dispersions lead to quasi-recrystallization.
  - At the critical dispersion, abnormal growth occurs.
- Measured properties used for low angle boundaries in Al, i.e. energy and mobility.
- Detailed analysis by Miodownik on subgrain structures with small mean misorientations: same result.
- Experiments by Ferry and Humphreys suggest that this behavior is observed experimentally.
Single Component + Dispersion (Mosaic Spread)
Small dispersion: 4° FWHM

Time = 1000 MCS  run name: cube26
Vf prtcls = 0.0000000E+00; size = 200
<r> = 2.659655  ; temp. = 0.1500000
prtcls = 0; no. bdry = 0
permtrs = 0; parts cnrns = 0
Intermediate dispersion: $8^\circ$ FWHM

Time = 1003 MCS  run name: cube30
Vf prtcls = 0.0000000E+00; size = 200
<r> = 2.669363 ; temp. = 0.1500000
prtcls = 0; no. bdry = 0
permtrs = 0; parts cmrs = 0
### Broad Dispersion: 13° FWHM

**Graph:**
- **X-axis:** Frequency (4°), Frequency (8°), Frequency (13°)
- **Y-axis:** Deviation (°), FWHM

**Data:**
- **Time:** 1001 MCS
- **Run Name:** cube35
- **Vf prtcls:** 0.0000000E+00; **size:** 200
- **<r>:** 2.676890; **temp.:** 0.150000
- **prtcls:** 0; **no. bndry:** 0
- **permtrs:** 0; **parts crnrs:** 0
Critical Dispersion

- Maximum area/\(A\) varies sharply with dispersion.
- Abnormal grains acquire larger misorientations.
Comparison with theory

Rollett & Mullins (1996); Miodownik (2001)

\[
\frac{dA}{dt} = -2\pi M\gamma \\
\Gamma = \frac{\gamma_{abnm}}{\gamma_{matrix}} \\
\mu = \frac{m_{abnm}}{m_{matrix}} \\
\rho = \frac{R_{abnm}}{\langle R_{matrix} \rangle}
\]

\[
a(\Gamma) = (6/\pi)\sin^{-1}(1/2\Gamma) < 3
\]

\[
\frac{d\rho_{abnm}}{dt} = \frac{M_{matrix}\gamma_{matrix}}{2\langle R_{matrix} \rangle^2} G(\rho, \mu, \Gamma)
\]

\[
G(\rho, \mu, \Gamma) = \left\{ \mu \Gamma \left[ a + (a - 2) \frac{1}{\rho} \right] - \frac{\rho}{4} \right\}
\]