Meso-scale Monte Carlo Sintering Simulation with Anisotropic Grain Growth

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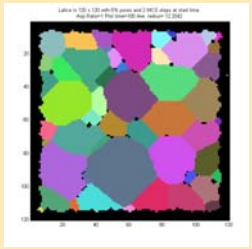
Introduction

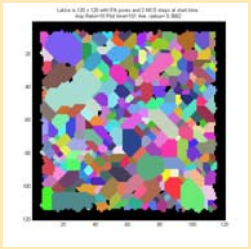
Sintering is a vital process in many industries, but how do the properties and dimensions change during sintering? To learn more about what happens during sintering, computer models are used to investigate the behavior of materials when sintered. One of the key issues is how grains evolve and grow.

Monte Carlo simulation models are one of the most common methods currently used to model this behavior. Very few of these models accommodate anisotropic materials which grow are a significant portion of real materials.

- Meso-scale models look at a small unit cell and simulate the driving mechanisms to determine how the grain structure will develop within the cell. These are typically simulated with Monte Carlo Potts Models.



Porous Isotropic MC Potts Model

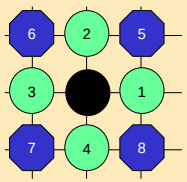


Porous Anisotropic MC Potts Model

The Potts Model

In 1925, Ernst Ising presented a two-state stochastic Markov Chain Monte Carlo model to sample the equilibrium distribution of ferro-magnetic domains. This was extended by Potts in 1952 for any number of states.

For energy calculations, only interactions with the nearest neighbors are considered.



$$E(C) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{8} E_{ij}$$

The distribution of energy states must satisfy the Boltzmann Distribution.

1st Nearest Neighbors

2nd Nearest Neighbors

The most commonly used algorithm to obtain a solution is the Metropolis Algorithm (1953) which uses an accept reject method with transition probabilities of

$$P_{accept} = \min\left(1, e^{-\Delta E / k_B T}\right)$$

Introducing Anisotropy

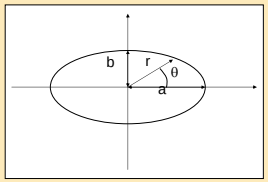
Many materials are anisotropic by nature, but in general, the Potts models do not capture the effects of anisotropy.

Anisotropy can be introduced into this model in the Jacobian used to calculate the energy change of a transition. In a 2-dimensional model, there are two components of surface energy, and then there is binding energy.

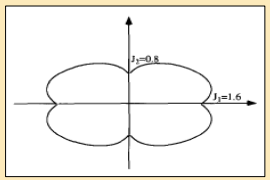
$$E_{ij} = \begin{cases} 0 & q_i = q_j \\ J_i + J_j + J_b & q_i \neq q_j \end{cases} \text{ where } \begin{array}{l} J_i \text{ and } J_j \text{ are surface energies} \\ \text{and } J_b \text{ is the binding energy} \end{array}$$

The misorientation between adjacent grains has a significant effect on the binding energy; but to start out, assume that the grain boundaries are fully wetted, so that the binding energy variability is negligible compared to the surface energies.

Wulff plots can be used to capture the surface energy of anisotropic materials in either 2-D or 3-D. Although Wulff plots for real materials can be quite complex, we can introduce anisotropy with one of the simplest Wulff Plots, the 2-D ellipse.



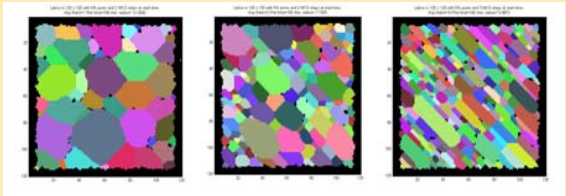
Ellipsoidal Wulff Plot



Two Cusp Wulff Plot

Anisotropic Growth

To visualize the effect of introducing anisotropy, start with aligned grain energies, and small isotropic grains.



Aligned grain orientations with Wulff plot aspect ratios (ar) of ar=1 (Isotropic Left), ar=2 (Middle) and ar=10 (Right)

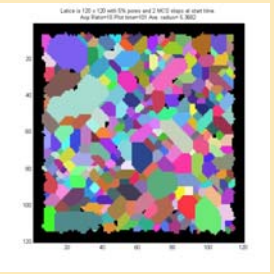
These structures all started the same, and ran for the same time. The only difference is the aspect ratios of the surface energy Wulff plots. Some observations follow:

- The Wulff plot aspect ratio affects anisotropy as expected.
- Increased anisotropy slows grain growth.

Random Orientation

Now let all grains be initialized with random orientations. In evaluating the results it is apparent that the lattice restricts growth in directions without a nearest neighbor.

One idea to overcome this artifact of the lattice discretization is to randomly rotate the lattice for each step of our simulation so that the effects of this artifact will be minimized.

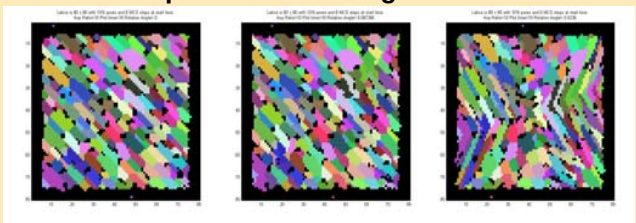


Rotation Algorithms

Algorithm requirements.

- Must be a one-to one mapping which maintains mass, porosity, grain size, etc.
- Some distortion and shifting of neighbors is necessary to get growth in non-neighbor directions.

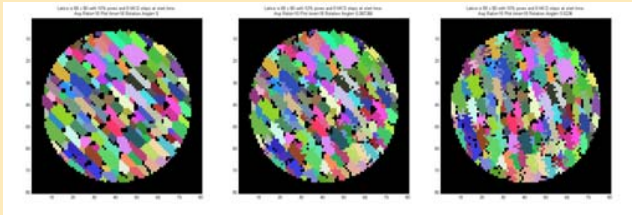
Square Rotation Algorithm



Rotation Angles of 0 deg (Left), 5 deg (Middle) and 35 deg (Right)

- Excessive distortion for large angles and large radii

Circular Rotation Algorithm



Rotation Angles of 0 deg (Left), 5 deg (Middle) and 35 deg (Right)

Further Work

- Quantitative comparison to other models and experiments.
- Incorporate misorientation angle effects on binding energy.
- Investigate templated grain growth.