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Simulation of abnormal grain growth in polycrystalline materials

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Abstract

Certain events of low probability that occur in material systems have a considerable impact on system characterization. Though rare event simulation has been a well-researched problem in areas like financial risk assessment and communication systems, modeling and simulation of rare events in material systems remain under-explored.

In this paper, we turn to large deviations theory and importance sampling to develop a solution to simulate an important rare event that arises in polycrystalline materials. More specifically, the microstructure of a polycrystalline material consists of grains that have different orientations associated with them. These grains evolve over time and this phenomenon is called grain growth. The growth of grains is a slow process, making direct observation expensive and impractical. To alleviate this problem, computational methods have been developed to simulate grain growth. However, one event of interest which occurs with low probability involves a single grain that grows abnormally large at the expense of other grains. Though Gibbs distribution based models exist for such abnormal grain growth, occurrence of this event under such models is still rare enough that we still need to draw many samples before an abnormal growth manifests.

We propose an importance sampling distribution from which to draw samples to simulate abnormal grain growth, instead of the conventional Gibbs distribution used to model grain growth. Our proposed importance sampling distribution is based on an asymptotically efficient rare event probability estimator. With our method, we consistently generate abnormal grain growth, thus providing a reliable solution to this important materials science problem. Our solution can potentially be used in general to simulate rare events in any system that is modeled by a Gibbs distribution.

Introduction

Several materials science phenomena that occur with low probabilities are crucial for designing reliable materials. An important example is a microstructure evolution phenomenon called *abnormal grain growth* in polycrystalline materials [10, 9]. It is a condition in which a few (typically one or two) "grains" (i.e., connected lattice sites of the same crystal orientation) grow abnormally big at the cost of other grains.

Modeling microstructure evolution with physical experimentation is a very slow process, making direct observation of grain growth expensive and impractical. Further, abnormal grain growth is considered to be a rare event, making it even more difficult to observe in a real material. This problem calls for accurate model-based simulation of microstructure evolution. Grain growth is sometimes modeled using a Gibbs distribution [10, 9], and can be simulated using Markov chain Monte Carlo techniques like the Metropolis-Hastings algorithm [15]. Though we can use Gibbs distribution-based models for simulating abnormal grain growth, occurrence of this event under such models is still rare enough that we need to draw many samples before an abnormal growth manifests. A solution to this problem is rare event simulation – a set of specific tools to simulate rare events [17, 4, 16, 19].

Rare event simulation has been a well-researched problem in areas like financial risk assessment [5, 6, 22], queueing and reliability modeling [2, 7], communication systems [18], and power system blackouts [23]. However, modeling and simulation of rare events in materials systems remain largely unexplored.

In this paper, we turn to large deviations theory and importance sampling to develop a solution to simulate abnormal grain growth. This solution builds upon the cohesive signal processing framework laid out for grain growth by Kubature et al. [12]. One of the most important considerations with respect to events like abnormal grain growth is how rare the event is. More specifically, we would want to know how rapidly the probability of this event falls toward zero as the size of the abnormal grain increases. To answer this and other questions, we first look at the theory of large deviations – an important branch of probability theory that is concerned with the asymptotic behavior of tails of probability distributions. More specifically, large deviations theory studies how fast the probability of certain events of interest falls to zero [21].

The rare event of abnormal grain growth can be seen as a large deviation from the expected grain growth patterns. If we assume that the probability measure associated with grain growth (modeled by a Gibbs distribution) obeys a large deviation principle [3], then we can use the rate function to propose another distribution in the Gibbs family under which the original rare event is more likely to occur. Sampling from this new distribution would consistently produce abnormal grain growth. The idea behind this solution to rare event simulation is called "importance sampling".

We set out to design an importance sampling distribution from which to draw samples to simulate abnormal grain growth. First, we turn to Bucklew's treatment to find a necessary and sufficient criterion to ensure an asymptotically efficient importance sampling density [4]. Then we invoke a powerful theorem from Baldi et al. [3] that gives the general form of an importance sampling density for a Gibbs distribution that satisfies the conditions outlined by Bucklew. This implies that our proposed importance sampling distribution leads to an asymptotically efficient rare event probability estimator.

Once we have the form of an asymptotically efficient importance sampling density for the Gibbs distribution, we choose an appropriate importance sampling potential that relates to the amount of abnormality in the microstructure. Application of the Metropolis-Hastings algorithm to draw configurations from such

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an importance sampling distribution would reduce the system energy while increasing the likelihood of an abnormal grain configuration.

What is Grain Growth?

Polycrystalline materials are made up of grains that have varying sizes and orientations. These grains undergo evolution under the application of heat and pressure. This process is known as grain growth (or more generally microstructure evolution). The growth of grains in a polycrystalline material is a very complex phenomenon and the factors that affect grain growth are not well understood. One approach to understanding the microstructure evolution is through computational simulation. In recent years, many computational methods have been developed to simulate grain evolution, and to study the effects of grain growth on the overall properties of a material. One such method uses the Potts model, with simulation based on Metropolis sampling[10, 1, 13]. The image processing community refers to the Potts models as a Markov Random Field (MRF). The MRF model can be written as a Gibbs distribution.

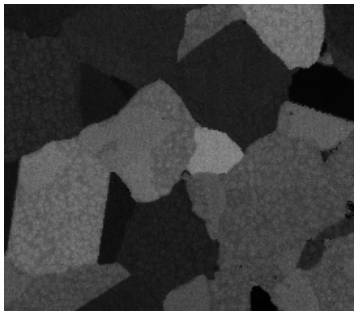

Figure 1. *Electron microscope image of a real polycrystalline material.*

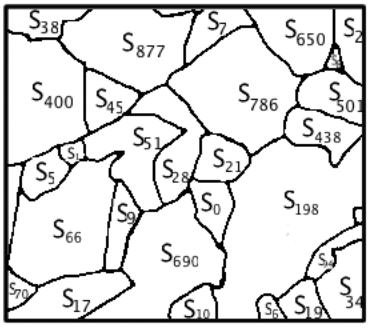

Figure 2. *Illustration of grain boundaries, with each grain labeled with an index representing its crystallographic orientation.*

Figure 1 shows an electron image of a real polycrystalline material. Figure 2 illustrates the boundaries between different grains. The label on each grain is an index indicating the crystallographic orientation of each grain.

In certain situations, one or more grains may grow abnormally compared to other grains in the system. This phenomenon is termed abnormal grain growth and it can be an undesirable, and sometimes catastrophic phenomenon. However, the occurrence of abnormal grain growth is stochastic, and relatively rare [8]. The purpose of this work is to model and simulate the event of abnormal grain growth using rare event simulation techniques.

Simulating Normal Grain Growth

Before we present our solution for simulation of abnormal grain growth, it is helpful to visit a state-of-the-art method for simulation of normal grain growth. We start with the Potts model and then describe how Metropolis-Hastings algorithm is adapted to simulate grain growth that is characterized by the Potts model.

Potts Model and Metropolis-Hastings Sampling

In this section we describe the simulation of the Potts model using a Metropolis method. The method presented in this section describes a technique to sample from a Gibbs distribution, which will later be adapted to the specific problem of grain growth.

Consider a system defined on an $n \times m$ lattice $L \subset \mathbb{Z}^2$ where each site in the lattice has one of Q possible orientations associated with it. Let $S = (S_1, ..., S_N)$ be a random configuration of orientation indexes on L, where S_i is an index that represents the orientation at site i, and $N = mn$ is the number of sites in the 2D lattice. Let $O_i = [\phi_i, \psi_i, \Theta_i]$ be the vector of Euler angles representing the crystallographic orientation at site i [14]. It should be noted that, due to the physics of grain growth, the number of possible orientations among grains in a polycrystalline material is finite.

Once we have assigned each lattice site j an orientation index S_j, we can define the notion of grains and related properties. A grain is defined to be a connected set of lattice sites, so that all lattice sites within a grain have the same orientation.

The energy of a configuration of orientations is often described by a Hamiltonian of the form,

$$E(s) = \frac{J}{2} \sum_{i=1}^{N} \sum_{j=1}^{z} (1 - \delta(S_i, S_j)), \tag{1}$$

where J is the energy associated with any pair of lattice sites with dissimilar orientation states, N is the total number of sites in the lattice, and z is the number of neighbors of each lattice site, and δ is the Kronecker delta function.

Assuming a Gibbs distribution, we can use the Hamiltonian of Eq. (1) to formulate the stationary distribution π from which to sample:

$$\pi(s) = \frac{1}{Z} \exp\left(\frac{-E(s)}{k_B T}\right), \tag{2}$$

where s denotes a possible configuration of the orientation states across all sites in the lattice, Z is the partition function, the interaction potential, $E(s)$, is the system Hamiltonian, k_B is the Boltzmann constant, and T represents the temperature.

Equations (1) and (2) represent the "Potts" model. To simulate the Potts model for grain growth [15], a lattice site i is chosen at random, and the orientation S_k of one of its unlike neighbors is selected as a potential new orientation for site i. The change in system energy corresponding to the new orientation at site i would be given by

$$\Delta E = E(s^{(i)}) - E(s^{(k)}), \tag{3}$$

where $s^{(i)}$ is the current lattice configuration and $s^{(k)}$ is the new lattice configuration with S_k as the new index at site i.

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If $\Delta E \leq 0$, then the orientation index of the given lattice site, S_i, is changed to the candidate orientation index S_k. If $\Delta E > 0$, then the orientation index at site is changed to the candidate index with probability $p(\Delta E) = \exp\left(\frac{-\Delta E}{k_B T}\right)$.

This is the simulation method based on the Potts model only. In order to more accurately model true grain growth, the method can be modified in accordance with domain knowledge to yield more realistic simulations [15]. This necessitates a clear mathematical outline of some properties of materials that make for useful simulation variables and parameters. This is described in the next section.

Grain Growth Simulation with Metropolis-Hastings Sampling

Boundaries between grains have important properties that have been shown to affect how the grains evolve. Holm et al. [9] discuss two important boundary properties relevant to this problem – boundary energy and boundary mobility, both of which depend on a scalar value called the misorientation angle. Given a boundary between sites i and j with unlike indexes S_i and S_j, we can define the misorientation angle as the smaller difference in angle between the orientations of the two grains on either side of the boundary. The misorientation angle between sites i and j is defined as the L^2 norm between the orientations O_i and O_j. That is, the misorientation angle θ_{ij} is given by,

$$\theta_{ij} = ||O_i - O_j||_2. \tag{4}$$

A grain boundary between sites i and j has a boundary energy γ_{ij} and a boundary mobility M_{ij}. These properties, which are both functions of misorientation angle θ_{ij}, are critical factors in grain growth. The boundary energy can be modeled by the Read-Shockley function [9] as,

$$\begin{aligned}\gamma_{ij} &= \gamma(\theta_{ij}) \\ &= \begin{cases} \frac{\theta_{ij}}{\theta_1}\left\{1 - ln\left(\frac{\theta_{ij}}{\theta_1}\right)\right\} & \theta_{ij} < \theta_1 \\ 1 & \theta_{ij} \geq \theta_1 \end{cases}\end{aligned} \tag{5}$$

The boundary mobility can be modeled by Huang and Humphreys equation [11] as,

$$M_{ij} = \begin{cases} 1 - \exp\left(-n\left(\frac{\theta_{ij}}{\theta_m}\right)^d\right) & \theta_{ij} < \theta_m \\ 1 & \theta_{ij} \geq \theta_m \end{cases}, \tag{6}$$

where n, d, θ_1, and θ_m are parameters that are experimentally determined. These two functions are plotted in Fig. 3 and Fig. 4, which show graphically how the energy and mobility of a boundary increase as the orientation difference between the grains increases.

Now, we redefine the total system energy (or Hamiltonian) to reflect the grain boundary energy of all grains that make up the system on the 2D lattice, as follows.

$$E(s) = \sum_{i=1}^{N} \sum_{j=1}^{z} \gamma_{ij}. \tag{7}$$

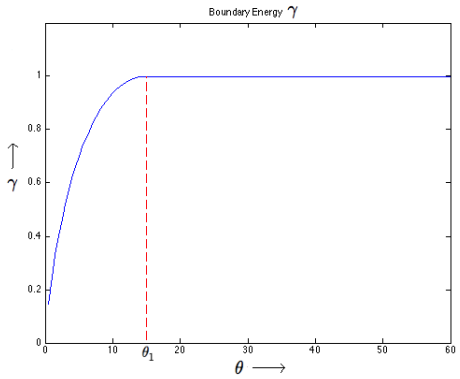

Figure 3. *Boundary energy as a function of misorientation angle. Here,* $\theta_1 = 15$ °.

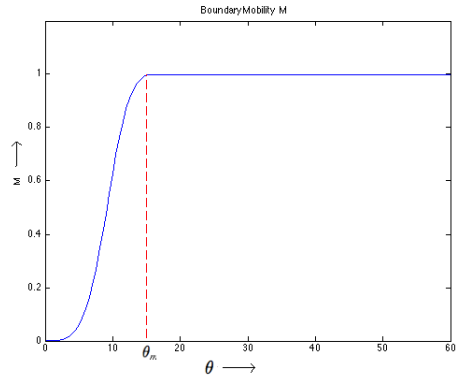

Figure 4. *Boundary mobility as a function of misorientation angle. Here,* $\theta_m = 15$ °, *n = 5 and d = 4.*

Also, we redefine the acceptance probability so as to induce a dependence on grain boundary mobility. This dependence is the link between this specific problem and the generic metropolis sampler.

$$\begin{aligned}&a(S_i^{(k+1)} | S_i^{(k)}) \\ &= \min\left(p_0, p_0 \exp\left(-\frac{(E(s^{(k+1)}) - E(s^{(k)}))}{k_B T}\right)\right),\end{aligned} \tag{8}$$

where $s^{(k)}$ and $s^{(k+1)}$ represent the lattice configurations where the i-th lattice site has an orientation index of $S_i^{(k)}$ and $S_i^{(k+1)}$, respectively.

Here, p_0 is the reduced mobility, given by,

$$p_0 = \frac{M_{ij}}{M_m} \tag{9}$$

where M_{ij} is the reduced mobility of the boundary between grains g_i and g_j, and M_m is the maximum reduced mobility in the system.

Grain growth is simulated using the Metropolis algorithm with the updated equations for the Hamiltonian, and acceptance probability as outlined in Eqs. (7) and (8) respectively. An outline of the Metropolis-Hastings algorithm is given in algorithm 1:

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Algorithm 1 Simulation in [15]

procedure EVOLVED GRAIN STRUCTURE ← SIMULATE(initial grain structure, max time)
    (Inputs: Initial grain orientation states, max time)
    (Output: Simulated grains, after growth modeled by Metropolis algorithm)
    while ($t <$ max time) **do**
        Choose a lattice site, i, at random.
        $S \leftarrow \{$all unlike states in the neighborhood of $i\}$
        $s(i)$ is chosen randomly from S
        Compute the change in the system energy, ΔE – resulting from this state reassignment.
        if $\Delta E > 0$ **then**
            Generate a random number $r \in (0,1)$.
            if $(r < p_0 \exp\left(\frac{-\Delta E}{k_B T}\right))$ **then** accept the new orientation state.
            end if
        elseAccept the new orientation state with probability 1.
        end if
        t++
    end while
end procedure

Theoretical Tools for Simulating Abnormal Grain Growth as a Rare-Event

One of the most important considerations when simulating events like abnormal grain growth is how rare the event is. In other words, we need to ask if the probability of the event to be simulated is very low. The notion of "very low" is vague and imprecise. Even if it were to be made precise, why should the simulation designer consider the rarity of the event? To answer these questions, we first look at the theory of large deviations – an important branch of probability theory that is concerned with the asymptotic behavior of tails of probability distribution sequences. After answering these questions using large deviations theory, we outline the theory of importance sampling that builds upon the foundations laid by large deviations theory.

Large Deviations Theory

Large deviations theory studies how fast the probability of certain events of interest falls to zero [21]. The "rate function" is a measure of the speed of the probability decay and will play a pivotal part in designing a density function from which to sample grain texture.

Before we start with the details, let us describe a simple fair-coin tossing experiment to explain the main ideas of large deviations theory. Though it does not concern microstructure evolution, this simple experiment serves our expository needs.

Let F be a random variable that records the outcome of a single toss of a fair coin. Then, F can take on two possible values,

$$F = \begin{cases} 0 & \text{if heads is tossed} \\ 1 & \text{if tails is tossed} \end{cases}. \tag{10}$$

The probability mass function for this experiment is given by,

$$p(F=0) = p(F=1) = 0.5. \tag{11}$$

Now, let us toss this coin n times. Suppose P_n is the probability measure associated with this experiment. Let $X = (F^{(1)}, F^{(2)}, ..., F^{(n)})$ be the outcome of the experiment and $T_n = T_n(X)$ be the average number of times tails is tossed.

$$T_n = \frac{1}{n}\sum_{k=1}^{n} F^{(k)}, \tag{12}$$

where $F^{(k)}$ is the outcome of the k-th toss (see Eq. (10)).

Suppose we would like to calculate the probability of the event $A = \{T_n > t\}$. We know, in this experiment, that $\mathbb{E}_p[T_n] = 0.5$. Therefore if $t > 0.5$, the event A would be a deviation from what is expected. Further, it would be reasonable to conclude that as $t - 0.5$ increases, the probability of event A under the measure P_n, $P_n(A)$, decreases.

Given a value of $t > 0.5$, the probability of event A, due to the WLLN, converges to 0 as $n \to \infty$, and this can be expected to generally decrease with increasing n. In addition to this behavior, if the deviation of t from the expected value increases, the probability, $P_n(A)$ decays. If this probability decay is exponential, then we say the sequence $\{P_n\}_{n\in\mathbb{N}}$ possesses a large deviations property. In case of the coin tossing experiment, the probability density function of the average number of tails has a large deviations property (see Fig. 5).

Mathematically, $\{P_n\}_{n\in\mathbb{N}}$ has a large deviations property if

$$\exists \text{ a function } I(A) \text{ s.t. } P_n(A) \approx \exp(-nI(A)). \tag{13}$$

The function $I(A)$ is related to the so-called rate function, $I(x)$, as follows,

$$I(A) = \inf_{x\in A} I(x). \tag{14}$$

The rate function associated with the coin-tossing experiment can be seen in Fig. 6.

The rate function, $I(x)$, is convex in x, and is defined through the Legendre transform [1] [20] as,

$$I(x) = \sup_{\theta}[\theta x - \phi(\theta)], \tag{15}$$

where $\theta \in \mathbb{R}$, and $\phi(\theta) = \lim_{n\to\infty} \frac{1}{n}\log(\mathbb{E}_p[\exp(\theta T_n)])$. The rate function, $I(x)$, achieves its minimum at $\mathbb{E}_p[T_n]$, which is 0.5 in this example.

[1] also called the Legendre-Fenchel transform.

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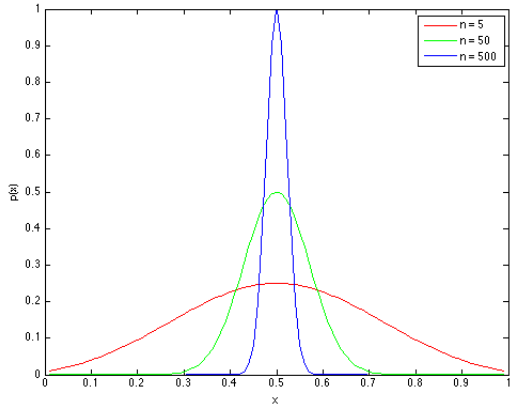

Figure 5. *Probability density function, $p(x)$, of the the average number of tails in a fair-coin tossing experiment. Here, n is the number of tosses.*

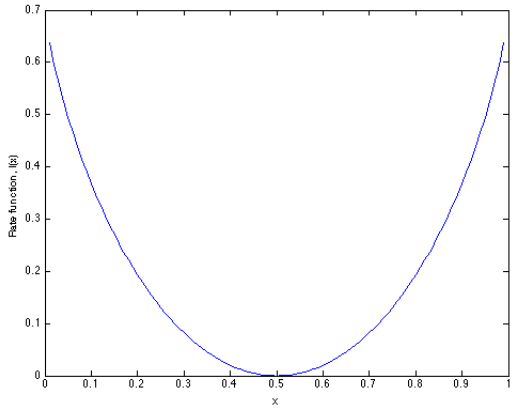

Figure 6. *Rate function, $I(x)$ for the fair-coin tossing experiment*

The idea of large deviations can be extended to any experiment. In the case of a Gibbs distribution, n takes the value of the lattice size instead of the number of independent trials (coin tosses, in our example). Intuitively, this means that the probability of a grain deviating from the "normal" (expected) size decays exponentially with the size of the material lattice, in conjunction with its own rate function. The next section deals with the question of simulating events that represent large deviations from the expected value of the random variable in question.

Importance Sampling

Suppose X is a random variable describing a random experiment on a sample space, with probability density given by $p(x)$. We are interested in evaluating the probability:

$$\rho = \mathbb{E}[\mathbb{1}_A(X)], \tag{16}$$

where, $\mathbb{1}_A(x)$ is an indicator function on the set A which is of interest to us. One way to evaluate Eq. (16) is to sample n i.i.d. random variables $X_1, X_2, ..., X_n$ from p(x) and calculate the estimate,

$$\hat{\rho} = \frac{1}{n}\sum_{i=1}^{i=n} \mathbb{1}_A(X_i). \tag{17}$$

Here, $\hat{\rho}$ is known as the Monte Carlo estimate of ρ. An alternative way to evaluate Eq. (16) is to sample n i.i.d. random variables $X_1, X_2, ..., X_n$ from a distribution $q(x)$ known as the importance sampling distribution, and to calculate the estimate,

$$\hat{\rho}_{IS} = \frac{1}{n}\sum_{i=1}^{i=n} \mathbb{1}_A(X_i)\frac{p(X_i)}{q(X_i)}. \tag{18}$$

Here, $\hat{\rho}_{IS}$ is known as the importance sampling estimate, and $q(x)$ is such that $\mathbb{1}_A(x)q(x)$ is non-zero for values of x at which $\mathbb{1}_A(x)p(x)$ is non-zero . We must choose the importance sampling density carefully. Ideally, the importance sampling density should be such that it hits the rare event of interest (A) more often. It can be seen that $\mathbb{E}_q[\hat{\rho}_{IS}] = \rho$, implying $\hat{\rho}_{IS}$ is an unbiased estimator of ρ.

We are now tasked with the problem of finding the criteria for a "good" importance sampling density. We turn to Bucklew's treatment to find a necessary and sufficient criterion to ensure an asymptotically efficient importance sampling density [4]. We begin by finding the variance of the estimator $\hat{\rho}_{IS}$:

$$\begin{aligned} n * var(\hat{\rho}_{IS}) &= \int (\mathbb{1}_A(x)\frac{p(x)}{q(x)} - \rho)^2 q(x)dx && (19)\\ &= \int \mathbb{1}_A^2(x)\frac{p^2(x)}{q(x)}dx - \rho^2 && (20)\\ &=: V_q - \rho^2 && (21) \end{aligned}$$

where, $V_q = \int \mathbb{1}_A^2(x)\frac{p^2(x)}{q(x)}dx$.

We want to minimize the estimator variance. Since variance is always non-negative, the minimum value that the variance can take is zero. With variance equal to zero, we get:

$$\begin{aligned} V_q &= \rho^2 \\ \implies \frac{1}{n}\log(V_q) &= \frac{1}{n}\log(\rho^2) \\ \implies \frac{1}{n}\log(V_q) &= \frac{2}{n}\log(\rho) \\ \implies \lim_{n\to\infty}\frac{1}{n}\log(V_q) &= \lim_{n\to\infty}\frac{2}{n}\log(\rho) \\ \implies R_q(A) &= 2I(A), \end{aligned} \tag{22}$$

where, $R_q(A)$ is the rate function associated with V_q, and $I(A)$ is the rate function associated with ρ. We consider Eq. (22) to be the necessary and sufficient criterion for an importance sampling estimator to be asymptotically efficient. Returning to our abnormal grain growth simulation problem, we can now work on picking an importance sampling distribution for the Gibbs distribution such that the criterion of Eq. (22) is satisfied.

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Importance Sampling for Gibbs Distribution

Formulating an importance sampling solution to the problem of microstructure evolution is, in principle, similar to that of the coin tossing experiment. However in practice, the underlying distribution, parameters of the model, and the physical experimental setting all make microstructure evolution a far more complicated problem than the coin tossing experiment. The differences, therefore, run deeper than the event of interest and the corresponding experimental outcome, necessitating a sophisticated simulation framework. A trial of this experiment consists of drawing a 2D sample (or configuration) from the Gibbs distribution, which is reproduced below:

$$\pi(s) = \frac{1}{Z}\exp\left(\frac{-E(s)}{k_B T}\right), \tag{23}$$

where the interaction potential, $E(s)$, is the Hamiltonian of configuration s as given in Eq. (7).

The function, T_n, is simply the fraction of the area occupied by the largest grain. $T_n : \mathbb{R}^n \to \mathbb{R}$, is a mapping from the n-tuple of all lattice sites on the 2D grid to a single real number. More formally,

$$T_n := T_n(s) = \frac{1}{n} \cdot \max_k \sum_{i=1}^{n} \mathbb{1}_{[g(i)=k]}(i), \tag{24}$$

where $g(i)$ gives the index of the grain to which the lattice site i belongs, and $k = 1, 2, ..., K$ is grain index, and K is the number of grains in the configuration s.

The event of interest, A, describes abnormal grain growth. So intuitively, it must correspond to the case where the largest grain has grown beyond a certain size (relative to the whole area). We can thus formulate A as:

$$A = \{s : T_n(s) > t\}, \tag{25}$$

where $t \in [0, 1]$.

With these foundations, we are now ready to formulate an importance sampling density for this problem modeled by the Gibbs distribution. We invoke a powerful theorem from Baldi et al. [3] that gives the general form of the importance sampling density for Gibbs distribution. We present a concise version of the theorem below:

Theorem 1 *An asymptotically efficient importance sampling density for the Gibbs distribution is guaranteed to exist. Further, the density function has the interaction potential given by,*

$$W(s) = E(s) - gG(s), \tag{26}$$

where $G(s)$ is any translation-invariant, absolutely summable interaction potential. The weight g can be found by solving the following equation:

$$\mathbb{E}_W[T_n(s)] = t, \tag{27}$$

where, $\mathbb{E}_W[\cdot]$ is the expectation taken with respect to the Gibbs density, π_W, with interaction potential given in Eq. (26)*, and configuration s is drawn from the importance sampling density, π_W.*

Using Theorem 1, it follows that an asymptotically efficient importance sampling density for Gibbs distribution is given by,

$$\begin{aligned}\pi_W(s) &= \frac{1}{Z}\exp\left(\frac{-W(s)}{k_B T}\right) \\ &= \frac{1}{Z}\exp\left(\frac{-(E(s) - gG(s))}{k_B T}\right).\end{aligned} \tag{28}$$

This importance sampling density satisfies the criterion in Eq. (22) and hence is asymptotically efficient. Now that we have the form of the importance sampling density for Gibbs distribution, it remains to choose an appropriate expression for the potential $G(s)$ that in some way relates to the measure of abnormality in the microstructure. Application of the Metropolis-Hastings algorithm would reduce the net potential, thereby reducing the system Hamiltonian while increasing the abnormality of the grain configuration. The balance between these two objectives is controlled by g, whose value we find by empirically solving Eq. (27).

An Importance Sampling Framework to Achieve Abnormal Grain Growth

In this section, we formulate an expression for the interaction potential, $G(s)$, and therefore, $W(s)$. For our purpose, G(s) must satisfy two conditions - it must be a measure of abnormality of the configuration, and it must have a form that can be summed over all the lattice sites in the configuration.

But what does it mean for $G(s)$ to measure the amount of abnormality in configuration s? A zeroth order approach would be for $G(s)$ to be a count of all sites in the configuration s that belong to the (most) abnormal grain [2] (with grain index k_{abn}). A better expression of $G(s)$ would not only count sites that belong to the abnormal grain, but also weight each count by *the abnormality of the neighborhood of each site*. The abnormality of the neighborhood could simply be a count of the number of neighboring lattice sites that belong to the abnormal grain. The second condition on $G(s)$ ensures that updating $G(s)$ (after every lattice site update in the Metropolis-Hastings algorithm) would be computationally tractable.

With these considerations in mind, our proposed expression for $G(s)$ is as follows,

$$G(s) = \sum_{i=1}^{N} c_i(n_i + 1), \tag{29}$$

where, N is the number of sites in the lattice,

$$c_i = \begin{cases} c_1 & \text{if site } i \text{ belongs to the } k_{abn}\text{-th grain} \\ c_2 & \text{otherwise} \end{cases}$$

c_1, c_2 are constants such that $c_1 > c_2$.

$n_i =$ number of neighboring sites of i that belong to the k_{abn}-th grain.

k_{abn} is the index of the most abnormally growing grain.

Note that the term $(n_i + 1)$ in Eq. (29) guards against the case when none of the neighbors of site i belong to the abnormal grain,

[2] This would raise the question of what would make a grain (the most) abnormal. We answer this important question after we develop an expression for $G(s)$, and we assume for now that we have a grain, $g_{k_{abn}}$, that is abnormally growing.

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as opposed to having just n_i which would zero out $G(s)$ even when site i belongs to the abnormal grain.

We calculate the index, k_{abn}, of the (most) abnormal grain by considering two factors:
(1) the size of the grains in configuration s, and
(2) the velocity at which the grains are growing.

Specifically, we compute the abnormal grain index by a very simple two-objective optimization as follows:

$$k_{abn} = \arg\max_k (s_k + w v_k^{(p)}), \tag{30}$$

where s_k is the size of the k-th grain, $v_k^{(p)}$ is its velocity, and the weight, w, balances the size and velocity. In order to make an assessment of how fast the grains are growing *currently*, we use the notion of "instantaneous" velocity. The (instantaneous) velocity, $v_k^{(p)}$, of grain k can be defined as the net growth of the grain k in the past p attempts [3].

Now that we have an expression for $G(s)$, we use it in conjunction with $E(s)$ (see Eq. (7)) in the Metropolis-Hastings algorithm as shown in algorithm 1 to simulate abnormal grain growth.

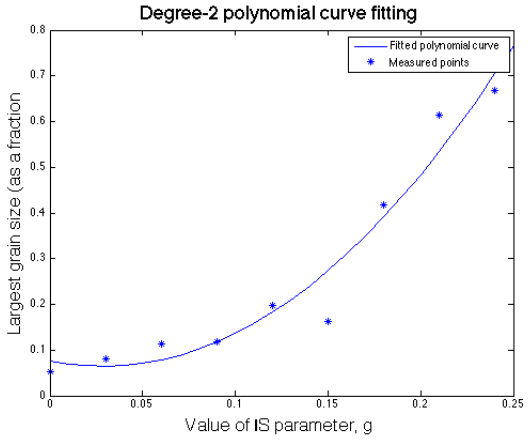
Putting all results together, the importance sampling density π_W (of Eq. (28)) can be explicitly written as,

$$\pi_W(s) = \frac{1}{Z} \exp\left(\frac{-\left(\sum_{i=1}^{N} \sum_{j=1}^{z} \gamma_{ij} - g \sum_{i=1}^{N} c_i (n_i + 1) \right)}{k_B T} \right). \tag{31}$$

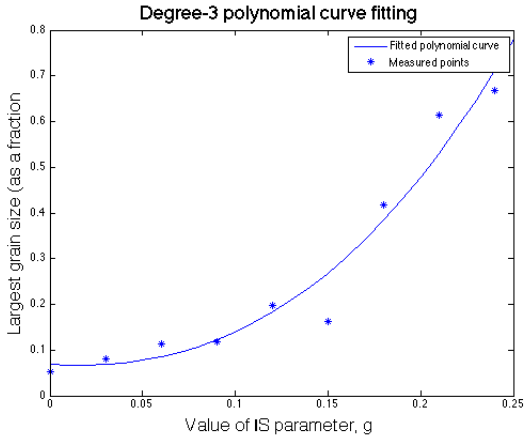
Results

We perform nine simulations[4] by varying the value of the importance sampling parameter, g (see Fig. 8, for representative examples). In order to observe the effect g has on the microstructure evolution, we keep other parameters (velocity weight w, c_1, and c_2) fixed. Specifically, we set $c_1 = 1$, $c_2 = -1$, and $w = 0.8$. We then vary g from 0 to 0.24 in steps of 0.03. The case where $g = 0$ corresponds to having no importance sampling potential term ($G(s)$), and our simulation falls back to the regular Monte Carlo framework. For each simulation s, we report the fraction of the area occupied by the largest grain.

In our experimental results, we observe that the largest grain size increases with increasing values of g. This property helps us solve for the required value of g empirically, given the knowledge of desired value of the largest grain size. Since we experiment with a limited number of g values, we perform a curve fitting operation to establish the relationship between g and the largest grain size. Specifically, we fit two polynomials (of degrees 2 and 3) that fit the data best (in the least squares sense), and the resultant curves are given in Fig. 7. While there is not much visual difference between the two curves, the 3rd degree polynomial curve represents a bijective function, and is therefore the more useful curve in determining the required value of g for a desired value of the largest grain size.



(a) Curve fitted to polynomial of degree 2



(b) Curve fitted to polynomial of degree 3

Figure 7. *Curve fitting to establish an empirical relationship between the desired values of the largest grain size and the corresponding required value of parameter g.*

The curve fitted to a polynomial of degree 2 is given by,

$$p_2(g) = 14.4360g^2 - 0.8508g + 0.0768. \tag{32}$$

and the curve fitted to a polynomial of degree 3 is given by,

$$p_3(g) = 17.4585g^3 + 8.1510g^2 - 0.2820g + 0.0689. \tag{33}$$

Conclusion

In this paper, we used large deviations theory and importance sampling to propose a simulation algorithm to simulate an important rare event that arises in materials science. Specifically, the phenomenon we dealt with was abnormal grain growth in polycrystalline materials.

We proposed an importance sampling distribution from which to draw samples to simulate abnormal grain growth, instead of the conventional Gibbs distribution. The proposed importance

[3] The value of $p = 1$ would be make the velocity highly instantaneous, but is not usually the best choice because of possible fluctuations. On the other hand, a high value of p makes the velocity less instantaneous and possibly "misleading".

[4] We modified Sandia National Laboratory's SPPARKS toolbox for our simulations.

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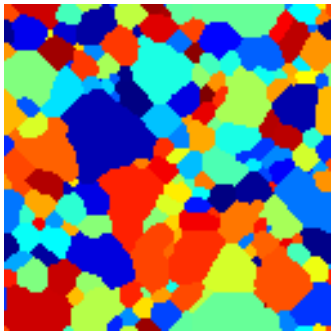
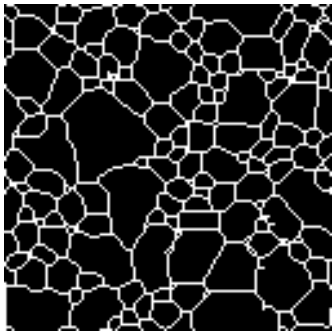
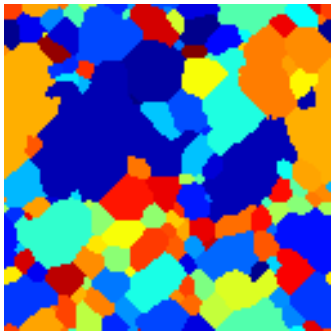


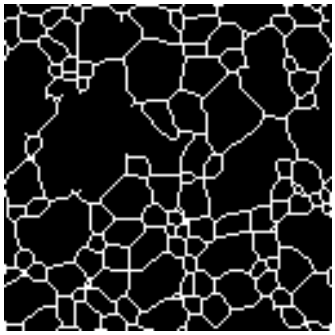
(a) Grains evolved after 20,000 MCS



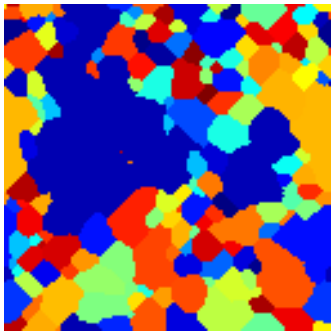
(b) Grain boundaries corresponding to (a)



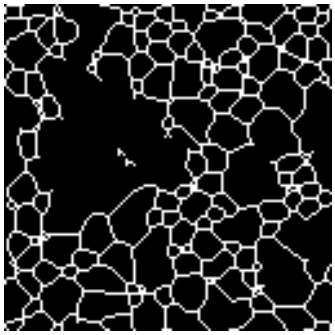
(c) Grains evolved after 20,000 MCS



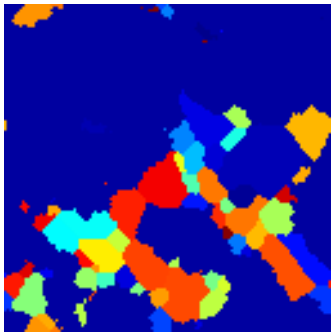
(d) Grain boundaries corresponding to (c)



(e) Grains evolved after 20,000 MCS



(f) Grain boundaries corresponding to (e)



(g) Grains evolved after 20,000 MCS

(h) Grain boundaries corresponding to (g)

Figure 8. *(a), (b) $g = 0.00$: regular (non-importance) sampling; largest grain size (relative to full area) = 0.052; (c), (d) $g = 0.06$; largest grain size (relative to full area) = 0.114; (e), (f) $g = 0.12$; largest grain size (relative to full area) = 0.198; (g), (h) $g = 0.24$; largest grain size (relative to full area) = 0.667.*

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sampling distribution is based on an asymptotically efficient rare event probability estimator. With our method, we have been able to consistently generate abnormal grain growth, thus providing a reliable solution to this important materials science problem. This work resulted in a general framework to simulate rare events in any system that can be modeled by the Gibbs distribution.

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