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Kinetics and anisotropy of the Monte Carlo model of grain growth

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Abstract—The Monte Carlo model is one of the most frequently used approaches to simulate grain growth, and retains a number of features that derive from the closely related Ising and Potts models. The suitability of these features for the simulation of grain growth is examined, and several modifications to the Hamiltonian and transition probability function are proposed. The resulting model is shown to not only reproduce the usual behaviors of grain growth simulations, but to substantially reduce the effect of the underlying pixel lattice on the microstructure as compared to contemporary simulations.
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1. Introduction

The Monte Carlo (MC) method is one of the main computational approaches used in the study of grain growth and related phenomena, and has provided useful qualitative insights into these processes for several decades. Derived from the Ising and Potts models of ferromagnetic systems, MC models represent a material as a collection of area or volume elements endowed with spins and arranged on a regular lattice. A grain is defined as a contiguous collection of material elements with the same spin, and the microstructure is evolved by probabilistic rules to propagate the spin of a given element to the neighboring ones.

Originally formulated in the context of microstructure evolution by Anderson et al. [1], the MC model quickly proved useful in the study of the grain growth microstructure [2], of stagnation in the presence of second-phase particles [3], of the effect of anisotropic boundary energies [4], and of the factors leading to abnormal grain growth [5–7]. Furthermore, the relative simplicity of the formulation allowed various implementations of the model to be extended for other purposes as well. For example, three-dimensional versions have been used to investigate the variations in grain structure around welds [8] and the effect of texture and texture evolution during grain growth on the microstructure [9], to evaluate a mean-field theory for the grain size distribution [10], and to support an analytical model for disordered cellular structures inspired by thermodynamic considerations [11].

Certain modifications of the underlying algorithm have been proposed to improve the computational efficiency of the model. The most important of these is the kinetic MC method, occasionally known in the materials science literature as the *n*-fold way algorithm. The fundamental observation is that using a variable time step equal to the interval required for the system configuration to change is often more efficient than using a constant time step and repeatedly proposing changes that may be rejected. While initially developed for the Ising model [12], the same approach may be applied to the MC model of grain growth [13]. This has the additional advantage that the kinetic MC method is readily parallelized [14,15], allowing the simulation of statistically significant volumes of material.

Unfortunately, the standard formulation of the MC model should not be used if predictive simulations of material behavior are required [16]. There are three main reasons for this assertion. First, the probabilistic rules used by the Monte Carlo method to update the system configuration do not have any physical basis. When initially formulated by Metropolis et al. [17], the purpose of the MC method was to model the distribution of states of a microscopic system in thermodynamic equilibrium. The rule for changing the configuration was chosen on the basis of mathematical simplicity, subject to the condition that the system sample states are at frequencies consistent with the canonical ensemble. By contrast, a microstructure is a macroscopic system far from thermodynamic equilibrium. A change of configuration is interpreted as grain boundary migration and should be subject to the corresponding

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kinetics, not to relations defined only for mathematical convenience.

Second, the quantities appearing in MC models do not have well-defined units, precluding the direct comparison of simulation results with experiments. For example, material elements have arbitrary spatial dimensions, time is measured in arbitrary units, and the temperature appearing in the Metropolis dynamics is meaningful only in the context of the type of simulations performed by Metropolis et al. [17]. This situation is caused by the absence of any suitable kinetic relations in the formulation of the model. While at least one analytic [18] and several numerical [19,20] approaches to assign units to the simulations have been proposed, none appears to have been widely adopted by the computational materials science community.

Third, the use of a lattice of material elements introduces an inherent anisotropy into the simulations. This causes various unphysical phenomena, including grain boundary faceting, deviations of the dihedral angles along triple lines, and grain growth stagnation. The consensus in the literature [21–24] seems to be that the anisotropy may be mitigated by carefully selecting the underlying lattice, by using a fictitious temperature high enough to introduce limited grain boundary roughening, or by increasing the interaction cutoff distance between material elements. None of these is entirely satisfactory though. The number of available lattices is limited, the temperature must be calibrated to balance the effects of unphysical boundary faceting with unphysical boundary roughening, and increasing the interaction distance dramatically accelerates the disappearance of small microstructural features.

The primary purpose of this paper is to reduce the inherent anisotropy of the MC model. Since the absence of a physical basis for the standard MC model means that nothing is sacrosanct, we make two modifications to the underlying algorithm. First, the strength of the element interactions is allowed to vary as a function of the element separation, rather than being a constant for all elements within the cutoff distance. Second, the configuration is updated by choosing one of several proposed configurations with a function that depends smoothly on the energy change, rather than accepting or rejecting a single proposed configuration with a function constructed only for mathematical convenience.

The performance of the modified MC model is compared to that of a standard MC model by analyzing the microstructures resulting from grain growth simulations. Specifically, we consider the distribution of grain boundary normal directions and the deviations of the rate of change of grain areas from the von Neumann–Mullins relation [25,26]. Comparing these with corresponding quantities for a truly isotropic material reveals that the modified MC model reduces the inherent anisotropy of the lattice significantly more than the standard MC model, and is therefore preferable to the standard MC model in practice.

2. Traditional Monte Carlo

The history of the MC method is briefly reviewed, with particular emphasis on the source of the algorithm. This will help to identify a set of features that may safely be changed without violating any fundamental mathematical or thermodynamic constraints, and serves as motivation for the modifications to the algorithm proposed in Section 3.

2.1. Ising and Potts models

The Ising and Potts models are mathematical models most often used to study phase transitions in ferromagnetic systems, and have a long history in statistical physics [27]. Assume that a regular lattice of particles endowed with magnetic spins inhabits a two-dimensional (2-D) region with periodic boundary conditions. The spin of a given particle interacts magnetically with the spins of neighboring particles, and possibly with an external magnetic field.

The study of this system is usually restricted to the expected distribution of states in the canonical ensemble. The interaction of neighboring particles effectively precludes an analytical solution, however [28], meaning that the expected distribution of states is usually evaluated by sampling as a given configuration moves through the state space. A set of rules to guide the evolution of the initial configuration is provided by either Glauber dynamics [29] or Metropolis dynamics [17].

The Ising and Potts models (and MC grain growth models) are customarily described within the framework of the Metropolis algorithm. This means that the usual formulations have the following three features:

1. The Hamiltonian provides the energy of a configuration of the system. It is generally constructed from the sum of finite-range pairwise interactions and should be non-negative, bounded and translation invariant.
2. The proposal distribution is the conditional probability distribution of the proposed configuration of the system in the following time step, given the current system configuration. It is often assumed to be a uniform distribution on the adjacent states in the configuration space.
3. The acceptance distribution (often known as the transition probability) is the conditional probability to accept the proposed configuration of the system in the following time step, given the current system configuration.

These three features of the Ising and Potts models will be described in further detail below to help clarify the historical underpinnings of the MC grain growth model.

The Hamiltonian used by the Ising and Potts models in the absence of an external magnetic field is most often of the form:

$$H = \frac{1}{2}\sum_i J \sum_j (1 - \delta_{s_i s_j}), \tag{1}$$

where the outer sum is performed over all spins, J is the energy penalty between spins of different orientations, the inner sum is performed over the spins in a standard neighborhood around the ith spin, and $\delta_{s_i s_j}$ is the Kroneker delta, equal to one whenever the states s_i and s_j of the ith and jth spins are the same and to zero otherwise. Notice that the energy of a configuration with all spins aligned is zero, and that the energy penalty for spins of different states is halved in Eq. (1) because of double-counting.

The inner summation in Eq. (1) will be called the kernel of the Hamiltonian, while the coefficient of the kernel will be called the energetic coefficient and the argument of the inner summation will be called the weighting function. The kernel is distinguished by being closely related to the change in the energy of the system when the state of a single spin is changed. Specifically, changing the state of the ith spin changes the system energy by:

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