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Editor's Choice

Strain energy limitations in Monte Carlo Potts modeling of grain growth

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ABSTRACT

Previous literature reports that the Monte Carlo Potts (MCP) method can only reproduce the linear relationship between grain boundary velocity and strain energy driving force expected under ideal grain growth conditions for small values of strain energy. The exact range of strain energy values for which linearity can be reflected in MCP are not defined. To determine this range, a series of simulations are performed using Monte Carlo Potts in both square 2D and cubic 3D geometries using the Moore neighborhood. These simulations consider cases in which strain energy is either the sole driving force for grain growth or coupled with grain boundary curvature. The 2D results show that the strain energy upper bound is approximately 3.5 non-dimensional units. The 3D simulations show that the relationship between grain boundary velocity and strain energy is dependent on grain boundary curvature. Grain boundary curvature can affect the upper bound of the range of strain energy and can impose a lower bound as well, below which grain growth is discontinuous or stagnate. Both 2D and 3D results are dependent on simulation temperature, with simulation temperature capable of altering the lower and upper bounds in 3D. Increasing simulation temperature in 3D decreases both the upper and lower linearity bounds. MCP simulations using simulation temperatures of zero are not suitable for modeling strain energy driving forces, as grain boundary velocity becomes discontinuous with strain energy.

1. Introduction

There is a variety of computational tools available to model mesoscale microstructural evolution. These tools can be broadly categorized as either continuum models: phase field models and vertex models, or discrete models: Monte Carlo Potts (MCP) and Cellular Automata (CA). Traditionally MCP and CA have been used to model different microstructural phenomena [1]. MCP is typically used to model curvature driven grain growth [2,3] while CA tends to be preferred to model recrystallization [4,5]. Both MCP and CA involve discretization of the microstructure into a lattice and simulate microstructural evolution by switching the grain that a lattice unit belongs to. The main difference between MCP and CA is the way they perform the switch. MCP performs lattice unit switching by evaluating the local system energy of a specific lattice unit and changing the grain the lattice unit belongs to if it will lower the system energy. CA performs lattice unit switching by evaluating whether the neighboring grains have recrystallized and switching the lattice unit to one of its recrystallized neighbors. Additionally, MCP lattice switching is stochastic, using a randomly generated number to determine whether a lattice unit should switch, whereas the standard form of CA is deterministic. The other key difference between the two models is the manner in which the microstructure is updated. MCP updates the progression of the microstructural evolution every time a lattice unit changes to another grain, but CA updates the entire microstructure at once. An entire sweep of the lattice for MCP is equivalent to a single lattice update for CA. Some models have been developed that blur the distinction between MCP and CA. These models incorporate the stochastic nature of MCP into CA, which will allow CA to model curvature driven grain growth [6].

Utilization of pure MCP [7,8] to model recrystallization has waned in favor of CA [9,10] including a few MCP/CA [11,12] hybrid models. The disaffection likely originates from literature reports indicating that MCP cannot model strain energy driven grain growth as well as CA [11,1]. An important requirement of computational models is the ability to reproduce fundamental theory for a prescribed set of assumptions. For curvature driven grain growth under idealized conditions, this amounts to a linear relationship between grain boundary velocity (V) and driving force (P): $V = MP$ (M is the grain boundary mobility), log-normal grain size distribution and classical grain growth kinetics: $d^2 - d_0^2 = kt$, where d is the instantaneous average grain diameter, d_0 is the initial grain diameter, k is a constant and t is time. For other driving forces under idealized conditions, there is only the expectation that

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$V = MP$. The verification of numerical models includes testing their ability to reproduce these expected outcomes under the same ideal conditions. The problem with MCP and strain energy driving forces is that the relationship between grain boundary velocity and strain energy driving force is nonlinear at large strain energies. Interestingly, the drop in MCP usage for recrystallization has occurred despite the lack of a curvature driving force in the standard form of the CA recrystallization model, or in the case of a stochastic CA model, a non-proportional relationship between the switching probability and strain energy [11]. MCP is capable of reproducing fundamental theory when subjected to curvature driven grain growth.

Hybrid models have been developed to address the weaknesses in both MCP and CA models. The work by Rollett and Raabe [11] proposes a hybrid model and simulates a simple static recrystallization problem to examine its kinetics. The recrystallization problem simulated involved seeding strain-free nuclei into a uniformly strained 2D microstructure, and allowing these nuclei to grow until the microstructure fully recrystallized. The kinetics from the simulation demonstrate that site-saturated Johnson–Mehl–Avrami-Kolmogorov (JMAK) [13] kinetics were recovered. The work by Madison et al. [12] proposes a different version of the MCP/CA hybrid model, and applies it to a dynamic crystallization problem. In this work a 2D microstructure continuously and uniformly accumulates strain energy. Nucleation attempts are made to a fraction of the microstructure and nucleation is successful if a critical strain energy value is exceeded. The newly nucleated grains can then grow by depletion of strain energy. These simulations progress for a set amount of simulation time. The pertinent information obtained from these simulations involve the time evolution of grain size and system energy. Results obtained by Madison and co-workers show that the grain size and system energy oscillate initially to then reach steady state. Recrystallization kinetics were determined for this hybrid model under the aforementioned circumstances and was found to also agree with JMAK predictions. Both hybrid models gave JMAK predicted recrystallization kinetics, however JMAK predictions involve homogeneous nucleation and are very idealized. Matching JMAK predictions under idealized conditions is good for model verification, but recrystallization is a heterogeneous process so JMAK kinetics rarely coincide with real materials [9]. Deviating from the JMAK predictions is a necessity when modeling real materials. The method to incorporate both MCP and CA in these hybrid models is to divide the microstructural evolution between MCP and CA depending on the situation. Recrystallization is governed completely by the strain energy driving force and is performed by CA, and grain growth is governed completely by the curvature driving force and is performed by MCP. The hybrid model proposed by Rollett and Raabe differentiate recrystallization from grain growth by comparing the magnitude of the strain energy driving force against the curvature driving force. Whichever driving force is greater determines whether CA or MCP is used. Both MCP and CA processes occur simultaneously. The hybrid model proposed by Madison et al. performs recrystallization and grain growth sequentially. 100 time steps of CA is performed before a single time step of MCP. Since the process simulated by Madison et al. is a dynamic one, there can be multiple waves of recrystallization occurring simultaneously, which is why they change the CA algorithm to be based on an energy minimization.

Hybrid MCP/CA models combine the features of each model that work well, however the two driving forces are still treated separately. The weakness of the hybrid models is that curvature and strain energy cannot be considered together to advance the microstructure's evolution. This leaves these hybrid models incapable of modeling situations where the two driving forces are in competition. Such situations include the presence of anisotropic grain boundary mobility, pinning particles and the involvement of subgrains during recrystallization [14,15]. These situations are certainly possible during recrystallization in real engineering materials and have remained neglected. For situations with driving force competition, either a new type of hybrid model must be developed or a further evaluation of MCP is in order.

MCP has been shown to perform well for curvature driven grain growth simulations. It has also been used for recrystallization simulation and was reported to yield linear driving forces at low strain energies, below 1 non-dimensional unit of energy (n.d.) [11]. However, the range of strain energy values for which the linear relationship is maintained has not been clearly defined in the literature. In addition, strain energy limitations could vary based on the lattice geometry and dimension due to the changes in geometry and the number of possible grain boundary segments associated to a single lattice unit.

The objective of this work is to investigate the relationship that strain energy has with grain boundary velocity as predicted by MCP simulation and to define the range of strain energy values for which this predicted relationship is linear. This investigation is conducted in the context of grain growth but, as shown above, has direct relevance to the simulation of recrystallization dynamics using MCP.

2. Numerical model

An overview of the Monte Carlo Potts method is provided here for completeness. Various monographs and books provide detailed descriptions [16–18]. The MCP approach presented here departs somewhat from a more classical presentation in that it allows for strain energy effects. The Monte Carlo Potts method simulates microstructure development stochastically over a finite discretized domain composed of lattice units (LU) that are each assigned an orientation. When two neighboring LU share the same orientation they are defined as being within the same grain. Otherwise they are defined as being part of different grains and a grain boundary exists between them. Grain boundary motion occurs by deciding whether each LU should change its orientation to that of one of its neighbors as the domain is swept iteratively. When a LU does change its orientation to the orientation of its neighbor, then the grain to which the neighbor LU belongs has grown by one LU.

The decision to change the orientation of the selected LU is based upon the comparison between a random number η and the Metropolis probability transition function:

$$P = \begin{cases} 1 & \Delta E \leqslant 0 \\ exp\left(-\frac{\Delta E}{T_s}\right) & \Delta E > 0 \end{cases} \quad (1)$$

where P is the probability of a LU changing orientation, ΔE is the change in energy that would result from an orientation change of the LU considered and T_s is the simulation temperature, a non-zero parameter used to add disorder to the microstructure evolution and avoid numerical artifacts that can develop due to discretization [19]. This probability transition function was developed to minimize the system's energy. If $\eta < P(\Delta E)$ the new state is accepted [16].

The energy associated with a single LU is defined by Eq. (2).

$$E_i = U_i + \sum_{j=1}^{N}(1 - \delta(q_i, q_j)) \quad (2)$$

where E_i is the energy of the selected LU, U_i is the strain energy of the selected LU, N is the number of nearest neighbors, δ is the Kronecker delta function, q_i is the orientation of the selected LU and q_j is the orientation of one of the nearest neighbors.