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Grain boundary energy and curvature in Monte Carlo and cellular automata simulations of grain boundary motion

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Abstract—Monte Carlo and cellular automata simulations of grain boundary motion generally suffer from insufficient units of measure. This complicates the comparison of simulations with experiments, the consistent implementation of more than one driving force, and the development of models with predictive capabilities. This paper derives the proportionality constant relating the voxel interaction strength to a boundary energy, derives a formula for the boundary curvature, and uses the Turnbull expression to find the boundary velocity. Providing units of measure for the boundary energy and the boundary curvature allow Monte Carlo simulations and cellular automata simulations, respectively, to be subject to more than one driving force. Using the Turnbull expression to relate a driving pressure to a boundary velocity allows the remaining quantities in cellular automata simulations to be endowed with units of measure. The approach in this paper does not require any calibration of parametric links, but assumes that the voxel interaction strength is a Gaussian function of the distance. The proposed algorithm is implemented in a cellular automata simulation of curvature-driven grain growth.

Keywords: Computer simulation; Monte Carlo method; Cellular automata method; Grain growth

1. Introduction

Monte Carlo (MC) and cellular automata (CA) simulations comprise a group of computational methods that have been successfully used to study microstructure evolution by grain boundary motion [1–4]. Grain boundary motion is conventionally driven by the reduction of either the grain boundary energy or the stored strain energy; the former is usually modeled by curvature-driven boundary motion, while the latter is usually modeled by normal motion of the boundaries into the strained material.

MC and CA simulations of grain boundary motion share several defining characteristics. First, the microstructure is represented at a length scale above that of atoms and below that of grains by a set of discretized volume elements known as voxels. A variety of physical processes [5–8] may be conveniently modeled by manipulating variables attached to the voxels, with the representation otherwise remaining invariant. One consequence of the discretized representation is an inability to precisely reproduce the smooth surfaces appearing in physical microstructures. This leads to the second defining characteristic, namely, that the grain boundary energy is calculated by a sum of pairwise voxel interactions rather than by a sum of surface element contributions. Specifically, a kernel is defined such that two voxels separated by less than the kernel radius and belonging to distinct grains contribute to the overall system energy. This effectively spreads the grain boundary over the kernel region, and serves to mitigate the consequences of the discretized interfaces [9–11].

Despite the versatility and prevalence of MC and CA simulations, several complications generally prevent this group of methods from quantitatively predicting material behavior. That is not to say that every MC and CA simulation is subject to all these limitations, or that MC and CA simulations have not been used to predict certain types of material behavior. Instead, the assertion is that all the following points must be satisfactorily resolved before this group of methods will be suitable for the design of engineering materials. The relevant obstacles include:

1. Arranging the voxels on a regular lattice influences the evolution of the system [12,13]. This is visible in the form of faceting of grain boundaries, deviations of the dihedral angles along triples lines, and stagnation of grain growth. This is a particular concern for material properties that depend on the grain boundary plane inclination [4].
2. Simulations often do not adequately reproduce curvature-driven grain boundary motion. The pressure on a grain boundary may be expressed as a function of the mean curvature by means of the Young–Laplace equation [14]. The mean curvature of a discretized interface is difficult to measure though, particularly when the kernel radius is small [15,16].

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3. The effective grain boundary energy given by calculating a sum of pairwise voxel interactions is unclear. While increasing the kernel radius increases the number of voxel interactions, the effective grain boundary energy should remain invariant. This complicates the implementation of MC simulations with more than one driving force [17,18].
4. The physical meaning of units of length, time and energy in simulations is often unspecified. This appears to be partly due to the ambiguity in calculations of grain boundary curvature and energy, and partly due to the use of dynamical relations not relevant to the physical system. The absence of appropriate units precludes the meaningful comparison of simulations with experiments.
5. The transition rules governing the change of voxel state are often not physically justified. Deriving error bounds on the simulated behavior is difficult when the relationship of the rules to the physical system is not explicit. Rules selected for historical reasons do not necessarily generalize to include additional information about the microstructure.

The author is not aware of any prior literature that conclusively resolves all of these obstacles, despite several encouraging attempts [17,19,18]. The research community has invested considerable effort in this direction though, and a concise review of some of the relevant approaches is offered below.

MC models were developed from Ising and Potts models of ferromagnetic systems used in statistical physics [20]. Initially used to simulate grain growth by Anderson et al. [1], they have since been used to study a variety of material behaviors [21,22,7]. MC models may be recognized by having a transition rule that is identical to that used for sampling the distribution of states of a microscopic system in thermodynamic equilibrium [23], and by incrementing time after applying the transition rule to a single randomly selected voxel. All energies are expressed in units of k_BT, where T is the temperature of the canonical ensemble and is conventionally regarded as an adjustable parameter. Notice that the transition rule and the temperature do not have a clear bearing on the physical system being modeled. As a consequence, MC models generally do not resolve points three, four and five above.

Nonetheless, there are two main motivations for using this transition rule. First, raising the temperature effectively reduces all dependence of the grain boundary energy on boundary plane inclination. This helps to reduce the effect of the voxel lattice on the evolution of systems with a constant boundary energy [9,24,25], but obscures meaningful energy variations in systems with an inclination dependence. Second, the probabilistic nature of the transition rule encourages grain boundary roughening. Interface fluctuations diffuse along the boundaries and result in curvature-driven motion on average [26,27], though roughening may cause the fragmentation of small grains and complicates the calculation of the boundary plane inclination.

Given the advantages of the MC model, numerous authors have attempted to provide the simulations with appropriate units of measure. Raabe [28] and Nosonovsky et al. [29] assigned units of length and time by equating the observed boundary velocity with that of the Turnbull expression, and Zöllner [25] proposed setting the reduced boundary mobility by adjusting the simulation temperature. They did not address units of energy though, or establish the relevance of the Hamiltonian to the energy of the physical system. Lusk et al. [30,24,18] partially solved this by equating the effective grain boundary energy with the free energy of an interface in the Ising model [31]. While this appears to allow all quantities in the MC model to be assigned units of measure, the parametric links require extensive calibration, depend on the voxel lattice, and hold only for high simulation temperatures and low bulk energy densities.

CA models in computational materials science developed from studies of self-reproducing Turing automata and population evolution in mathematics [32]. Hesselbarth et al. [3,33] made the earliest use of CA models in materials science for several simulations of static recrystallization. This encouraged a relative proliferation of recrystallization studies [34–37], though the model has been used for other purposes as well [38,39,8]. CA models seem to include any simulation that represents the microstructure by a collection of voxels, that updates the voxel state using only local information, and that increments time after applying the transition rule to all voxels. This gives considerable flexibility to tailor the variables attached to the voxels and the transition rules to suit the application at hand. Specifically, modeling the transition rule on a phenomenological rule derived from experiments effectively resolves points four and five above.

Part of the historical emphasis on recrystallization studies is likely due to CA models having difficulty reproducing curvature-driven grain boundary motion. There is considerable historical precedent for the kernel to be smaller than is suitable for reliable boundary curvature measurements [40], and the transition rules in CA models do not usually allow the effect of curvature to be handled by grain boundary roughening. A related concern is that the boundary plane inclination is strongly affected by the voxel lattice [4,13]. This effect is more serious for CA models than for MC models since there is no adjustable parameter to reduce the grain boundary energy dependence on boundary plane inclination. As a result, the contribution of the grain boundary energy is often neglected entirely; this serves as a reasonable approximation provided there is enough strain energy to induce static recrystallization.

This situation is not inherent to the CA model though, and multiple proposals have been made to increase sensitivity to boundary curvature and reduce lattice anisotropy. Several authors [38,41,42] interpreted voxels as microscopic volumes with variable thermal energies, resulting in boundary roughening and curvature-driven boundary motion. This approach suffers from some of the same difficulties as the MC models. Lan et al. [43] explicitly calculated the boundary curvature by a template method and found the pressure on the boundaries with the Young–Laplace equation [14]. This allowed grain growth to be simulated, but the authors state that a more accurate method of measuring boundary curvature would be useful. Mukhopadhyay et al. [44] and Marek [12] reduced lattice anisotropy by subdividing the voxels and allowing partial voxel occupation, respectively, but do not mention the boundary energy. Janssens [19] made the dramatic move of distributing the voxels on a random grid. This not only completely removed the lattice anisotropy, but enabled simulations of simultaneous recrystallization and grain growth. Perhaps only the increased complexity of the algorithm discouraged this approach from being more widely adopted.

Finally, Rollett and Raabe [17] published a hybrid algorithm that randomly alternated time steps between an MC