



# Modelling and understanding materials microstructure evolution driven by interface energy



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## ABSTRACT

The importance of microstructure is clear from the large body of research made on quantitative analysis and modelling of microstructures. Many real materials have complicated topological and morphological features in their microstructure that are critical to their properties and functionality. Here it is shown that complicated microstructure changes of real materials driven by interface energy can be simulated by cellular automaton approach as the consequence of matter movement guided by interface energy differences. This has become possible by introducing a concept of “structural imbalance” which is used for the quantitative determination of the driving force for microstructure changes. The new modelling approach is used to simulate the grain growth and complicated morphological evolution of 2 dimensional particle coating. This approach aids in understanding microstructure evolution at a fundamental level. It can also be a more efficient modelling method capable of dealing with the complex topology and morphology of real microstructures.

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## 1. Introduction

Understanding the temporal and spatial evolution of the morphology or microstructure of materials is not only of fundamental interest to physicists and materials scientists, but also important in the processing and application of technologically advanced materials [1]. Many real materials have complicated topological and morphological features in their microstructure that are critical to their properties and functionality [2–5]. In order to be able to predict the behaviour of materials, it is necessary to predict the evolution of their microstructures, but this has proved to be an elusive goal [6].

Cellular automata (CA) related modelling techniques are powerful methods to describe, understand and simulate the behaviour of complex systems [7]. In CA, space is discretized and made up of cells. Each cell is characterized by an internal state. The system then evolves in discrete time steps, like simple automata, according to a set of rules whose output is a function of the states of the cell and its neighbours. CA can be compared to a synthetic model of the universe in which physical laws are expressed in terms of simple rules for cell state transition. It was found that even when the underlying rules are very simple, the behaviour they produce can be highly complex, and can mimic many features of what is observed in nature [8,9].

CA intrinsically retains important aspects of the microscopic laws of physics such as simultaneity of motion, locality of interaction and time reversibility [7]. Materials are made of atoms or molecules. Microstructure changes of a material are the natural result of atomic or molecular movements which, in turn must follow certain laws of physics.

So far CA have been used in modelling recrystallization [10–13], grain growth [14–16], and surface mass transportation [17,18], where specific circumstances have specific driving forces for microstructure change such as stored elastic energy, stored dislocation density and crystallographic orientation mismatch [19–21], thermal or compositional gradients. However, a more general driving force for microstructure change is reduction of total interface and/or surface energies. These driving forces exist in any material under any circumstance. An in-depth understanding of microstructure changes driven by this general driving force is critically important for materials science.

So far the CA transition rules used for describing the meso-scale dynamics driven by interface energy are mainly based on ‘cell-counting’ method [14,17,18,22]: for example for modelling grain growth, Liu et al. [14] used deterministic CA cell transition rule based on a simple cell-counting method: if three cells among the four surrounding cells have the same state as the cell in concern, the state of this cell will keep its original state at the next time step. Whereas other workers [17,18,22] proposed that the number of air cells in the neighbourhood of an interface cell can

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be an approximate measure of the local surface curvature of the cell in concern. While all these works imply that the ‘cell-counting’ method could be an efficient way of measuring the local curvature or interface energy, the exact physics meaning of the ‘cell-counting’ has not been clarified.

It is well known that unbalanced bonding at interface can lead to a higher free energy. In fact, attempts have been made to quantify the unbalanced bonding at interface for determining the interface energy based on pair-wise atomic interaction [23]. To determine the interface energy based on inter-atomic interaction would need the detailed structural information in molecular level, which is, in many cases, impractical in terms of the availability and computation cost. In the meso-scale modelling, however, the structural details in molecular level of material can be neglected and the properties within each cell can be regarded as being uniform. The unbalanced structure at interface can be quantified based on pair-wise interaction between meso-scale cells, which was found to be consistent with classic theory about the excess interface energy arising from the curvature [24,25]. The term ‘structural imbalance’ here is used to describe the quantified unbalanced structure at interface and used interchangeably with interface energy.

In this paper, firstly the meso-scale cell interaction model is introduced for quantification of structural imbalance for interface and surface cells. The dynamic evolution of the system then takes place by applying probabilistic transition rules. It is demonstrated that complicated microstructure changes driven by interface and surface energy can be reproduced by the CA model using a simple local transition rule based on well-established physical principles. For simplicity and convenience of presentation, only 2-D microstructure is modelled and presented in this work.

## 2. Interface energy

The driving force for relocation of the interface atoms is directly related to their excess energy level, which in turn determines the dynamic evolution of microstructure when combined with an available transport pathway. The interfaces have higher energy level because the environment of interface atoms differs from that of bulk atoms in that the interface atoms have unbalanced bonding. The imbalanced atomic interactions near an interface give rise to the higher energy and lower stability of interface atoms. Therefore the interface energy can be calculated by quantifying the local structural imbalance (i.e. the degree of imbalance of atomic interactions in local neighbourhood).

In CA modelling, the space is discretized into cells. Typically cell size can, although not necessarily, be much larger than an atomistic lattice. In a previous paper [25], the structural imbalance of interface cells quantitatively determined using pair-wise cell interaction model was shown to be linearly proportional to the curvature, which agrees with the classical continuum theory, but no detailed derivation of the equations was given in [25]. Here a more detailed description of 2 dimensional meso-scale cell interaction model is given in the following.

Any bulk cells which locate sufficiently far from any interfaces have a balanced interaction, therefore they do not have structural imbalance. Compared to a bulk cell, an interface cell has an un-balanced arrangement of cells in its neighbourhood. By analogy to interatomic Coulombic interaction, the “long range” interaction between two cells is defined as:

$$U_{ij} = C_o \frac{\delta_{c_i c_j}}{r_{ij}} \quad (1)$$

where  $U_{ij}$  is the interaction potential,  $r_{ij}$  is the distance (all the distance in discrete CA model is measured in units of cell size, instead

of actual physical length), and  $C_o$  is an interaction parameter between two contacting cells.  $\delta_{c_i c_j}$  is the Kronecker delta: when the two cells are the same (i.e.  $c_i = c_j$ , where  $c_i$  is the type of the cell at position  $i$  and  $c_j$  is the type of the cell at position  $j$ ),  $\delta_{c_i c_j} = 1$ , otherwise  $\delta_{c_i c_j} = 0$ .

For the determination of structural imbalance, only the interaction between different types of cell needs to be taken into account, because cells of the same type in the neighbourhood do not contribute to structural imbalance. Therefore, the structural imbalance of an interface cell can be quantified as:

$$U^x = C_o \sum_{i=1}^n \frac{\sum_{j=1}^{8i} C_{mis}^{ij} (1 - \delta_{c_x c_{ij}})}{V_i r_{ij}} \quad (2)$$

where  $n$  is the mask size (units of cell dimension, instead of physical length),  $\delta_{c_x c_{ij}}$  is the Kronecker delta,  $C_{mis}^{ij}$  is the mismatch coefficient between the cell  $c_{ij}$  and the target cell ( $c_x$ ); (mismatch between a condensed phase cell and a void cell is taken as 1, whereas that between different condensed phases or crystallite orientations is 0–1) and  $V_i$  is the “volume” enclosed by the  $i$ th layer (for 2-D case,  $V_i = (2i - 1)^2$ ; for 3-D case,  $V_i = (2i - 1)^3$ ). Therefore the above equation can be rewritten for 2-D case:

$$U^x = C_o \sum_{i=1}^n \frac{\sum_{j=1}^{8i} C_{mis}^{ij} (1 - \delta_{c_x c_{ij}})}{i(2i - 1)^2} \quad (3)$$

The relative structural imbalance with respect to the flat surface is defined as:

$$\Delta u^x = (U^x - U^f) / U^f \quad (4)$$

where  $U^f$  is the structural imbalance of a flat surface cell for 2-D (where  $C_{mis}^{ij} = 1$ ):

$$U^f = C_o \sum_{i=1}^n (4i - 1) / [i(2i - 1)^2] \quad (5)$$

Therefore the relative structural imbalance for 2-D case:

$$\Delta u^x = \frac{\sum_{i=1}^n [1 - 4i + \sum_{j=1}^{8i} C_{mis}^{ij} (1 - \delta_{c_x c_{ij}})] / [i(2i - 1)^2]}{\sum_{i=1}^n (4i - 1) / [i(2i - 1)^2]} \quad (6)$$

For a glassy phase or amorphous phase, the random variation in the cell interaction can be taken into account by replacing the Kronecker delta by  $\delta = 1 + P(0.5 - R)$ , where  $P$  is interaction energy variability (in percentage) involving cells of the same type, and  $R$  is a random value between 0 and 1.

Distinct interfacial atomic structure or composition profiles (complexion, segregation, or space charge) [26] may exist at an interface which leads to partial relaxation of the local structural imbalance. This would mean that cells near an interface could have different electronic structure from the bulk cells. However, these features typically have very short length scale (a few lattice parameters), whereas the size of a cell, is typically much larger than the lattice parameter. For simplicity, in what follows these subtleties are neglected. However, this does not affect the general applicability of the current model. If such factors as orientation dependence of the surface energy are known or obtainable from atomistic simulations, they can be incorporated into the algorithm for calculating the structural imbalance of the interface cells.

## 3. Grain growth

Grain boundary migration is a result of the atoms or molecules in one grain jumping across a GB to become part of the neighbouring grain. The difference in frequency between forward jumping and backward jumping can be expressed as [27]:

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