CELLULAR AUTOMATA MODELLING OF NANO-CRYSTALLINE INSTABILITY

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ABSTRACT

A cellular automata model of nano-grain instability is proposed. The model includes 3 steps: nucleation, solidification and competition. The competition stage implements a modified Gibbs-Thompson criterion to determine the direction and the magnitude of the grain boundary migration. The model predicts grain coarsening and abnormal grain growth. The model is freely available from http://seis.bris.ac.uk/∼mexas/cgpack/.

1   INTRODUCTION

Nano-crystalline materials offer a promise of increased strength. However, it has been observed that some heat treatments lead to instabilities which result in abnormal grain growth [1], with few grains reaching 100 times the average size. This dramatically reduces strength. This work is aimed at predicting the emergence of abnormal grains and their effect on properties of the bulk material.

Size scale is the key factor when modelling mechanical behaviour of materials. A range of models exist from 10^{-10}m molecular dynamics (MD simulations [2]) to 10^{-6}m crystal plasticity FE (CPFEM) [3]. MD is conceptually simple, but vast computer resources are needed to analyse even a cubic nanometre of a solid. On the other hand CPFEM usually involves tens of material parameters, which are hard to obtain experimentally.

One material modelling technique growing in popularity is cellular automata (CA) [4]. CA is a discrete space - discrete time approach. The strengths of the CA method are simplicity and scale independence. In this work a CA method is developed for the evolution of nano-grain microstructures and show how it can be applied to predicting abnormal grain growth.

2   CELL STATES, NEIGHBOURHOOD AND SOLIDIFICATION

The 3D model space, with self-similar boundaries, is partitioned into identical cubic cells with a square grid. A cell's state can be either 0 for the liquid phase or a positive integer denoting a particular grain.
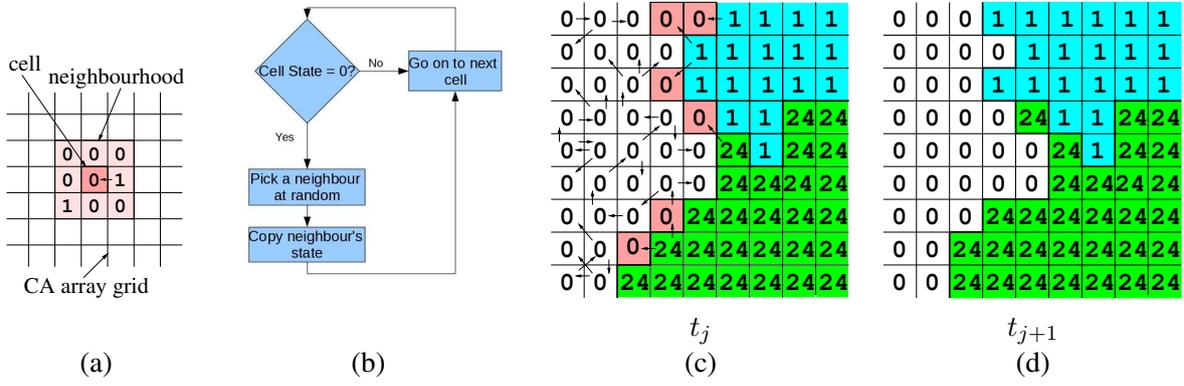
Figure 1: 2D sections of the 3D CA model, showing (a) a cell with its 8 nearest neighbours in a 2D slice (the other 18 neighbours are in the adjacent planes above and below the plane of drawing, and therefore not visible). The arrow indicates change of state of the central cell based on the state of a randomly chosen neighbouring cell. In this example the central cell had state 0, the liquid phase, and will have state 1 on next time increment, i.e. it will belong to grain 1. (b) A solidification flowchart. (c) A fragment of CA array at time t_j with 2 grains (1 and 24) and liquid phase (0). The arrows show change of state of the liquid cells. Note that each liquid cell will change state exactly once within one time increment, however the majority of changes are from liquid to liquid, i.e. having no effect. Only 6 liquid cells 'solidified', that is they became attached to solid grains in this fragment. (d) The state of the same fragment at t_{j+1}. Note the irregular grain boundary.

A grain is a collection of cells with the same state. For each cell a neighbourhood is defined consisting of 26 nearest neighbours ($3 \times 3 \times 3$ cube minus the central cell), shown in Fig. 1a. The state of each cell in the next time increment is a function of the state of the neighbourhood cells at the current time increment.

At the onset of the simulation a CA array with P cells is created. Initially all cells have state 0. Then the array is populated with N grain nuclei, $N \ll P$. Each grain nucleus is a single cell. Crystals with a cubic unit cell are assumed (i.e. BCC or FCC), and tie the grain coordinate system of each grain, X_i, $i = 1, 2, 3$, to its crystallographic directions: X_1 is [100], X_2 is [010], X_3 is [001]. Each grain is assigned a random orientation tensor, $\mathbf{R}$, such that $x_i = R_{ij}X_j$.

Each time iteration, all cells are scanned in turn, and if a liquid cell (state 0) is encountered, it is given a state of one randomly chosen neighbouring cell. This is shown schematically in Fig. 1b. The probability of a cell turning into any of its 26 neighbours is 1/26, i.e. any growth direction is equally likely. Fig. 1c-d shows a fragment of the CA array during a single solidification step.

Each grain expands outwards as a roughly spherical volume. The roughness of the resulting boundary is not only due to the voxel representation of the space but also due to the random nature of the solidification rule. In contrast, the geometrical polycrystalline models [3] typically assign crystallographic orientation and type to each grain boundary. It is very hard, if at all possible, to achieve this with the CA model.

The solidification stage is complete when there are no more liquid cells left.

Uniform random nucleation distribution results in equiaxed nano-structures, Fig. 2a. However, other grain structures are easily obtainable, e.g. a bi-modal grain structure results from seeding nuclei with different density in two halves of the CA array, Fig. 2b.

3 GRAIN COARSENING (COMPETITION)

Grain boundaries are regions of disrupted atomic lattice, with elevated elastic energy. Increasing grain sizes reduces the total volume of boundaries, thus lowering overall elastic energy. Therefore it is energetically preferable to change from smaller to bigger grains. This process is called grain coarsening. A modified Gibbs-Thompson equation [5] was used to implement this in the CA model:

$$\frac{\mathrm{d}r}{\mathrm{d}t} = M\gamma \left(\frac{1}{r_N} - \frac{1}{r} \right) \tag{1}$$

where r is the radius of the grain in question, r_N is the radius of a neighbouring grain, M is the boundary mobility and γ is the grain boundary energy.

Given two grains a and b, the grain misorientation tensor, $\mathbf{g}$, is defined as $\mathbf{g} = \mathbf{R}_a \mathbf{R}_b^T$. Then the grain misorientation angle, θ, is [6]:

$$\theta = \arccos \left(\frac{\mathrm{Tr}(\mathbf{g}) - 1}{2} \right) \tag{2}$$

By applying Eqn. (1) to all grain boundary cells grain coarsening was successfully simulated, including abnormal grain growth, Fig. 2c.

4 SCALING AND RESOLUTION SENSITIVITY

The ratio $\epsilon = N/P, \epsilon \in (0 : 1]$ is used as the model *resolution*, with $\epsilon \to 0$ meaning extremely high resolution and $\epsilon \to 1$ meaning very coarse resolution. The major output of the model is grain size distribution, Fig. 3b. Thus it was important to assess how much grain size distribution changes with ϵ.

This analysis was conducted with $N = 10^3$ grains and P from 5×10^6 to 4×10^8 cells. The grain sizes were normalised by the mean grain size. The standard deviation is shown in Fig. 3c as a function of ϵ (the grain density). The conclusion is that as long as the resolution is $\epsilon < 10^{-5}$, or more than 10^5 cells per grain on average, the model predictions are independent of the resolution. Using this limit, and assuming the mean grain size of 50 nm, the cell is approximately a $1 \times 1 \times 1$ nm cube. Given that atom sizes are in the order of 0.1 nm, a CA cell therefore represents 1000 atoms on average.

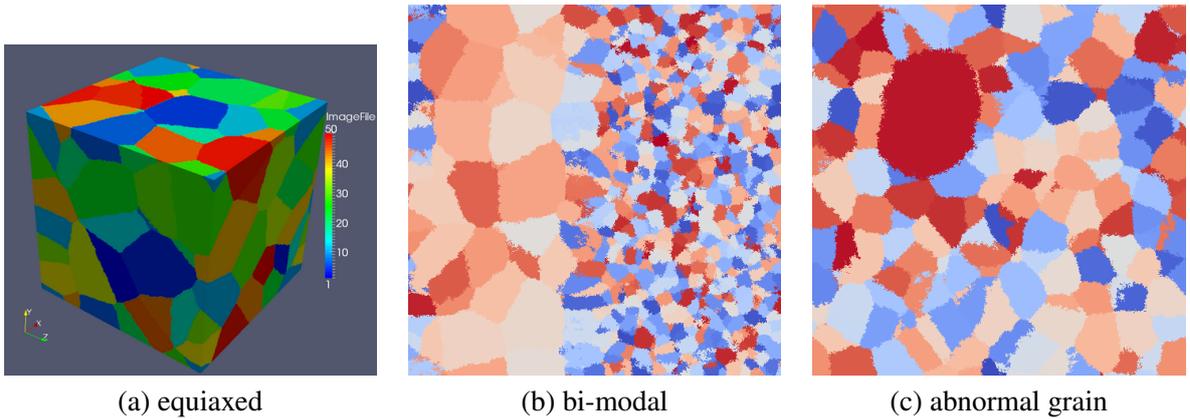| (a) equiaxed | (b) bi-modal | (c) abnormal grain |

Figure 2: Nano-structures produced (a) and (b) after the solidification step and (c) after the competition step. Colours are for ease of visualisation only, they do not denote grain orientation.
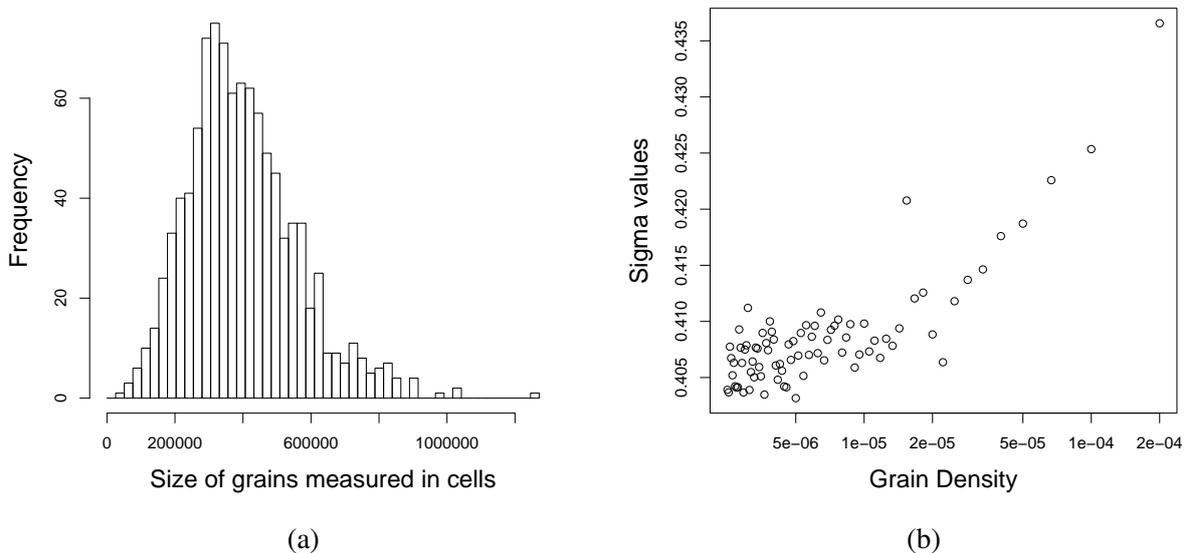
(a)   (b)

Figure 3: (a) Simulated grain size distribution, following a typical tailed distribution observed experimentally. Note that actual grain volumes were used, not equivalent circular diameters (ECD). The ability of our CA model to predict irregular grains and to calculate actual volumes is a major strength. (b) Change of standard deviation of grain size distribution with the resolution (grain density). Note the saturation behaviour, i.e. as long as $\epsilon < 10^{-5}$ the model predictions are virtually unchanged.

5 CONCLUDING REMARKS AND FUTURE WORK

It was demonstrated how a CA model can be used to predict nano-structures and their evolution, including abnormal grain growth, using a simple Gibbs type relationship. One useful application of the CA nano-grain model is simulation of fracture in nano-grain structures, e.g. using the CAFE multi-scale approach [7]. This is another direction for further study. Finally, parallelisation of the three nested cell update loops with OpenMP will be attempted. In future parallelisation with with MPI, or using fortran2008 `co-array` feature will be explored, to simulate models with more grains at high resolution.

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