Materials and Design 55 (2014) 740–746

Contents lists available at ScienceDirect

Materials and Design

journal homepage: www.elsevier.com/locate/matdes

Monte Carlo simulation of polycrystalline microstructures and finite element stress analysis

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ARTICLE INFO

Article history:
Received 11 July 2013
Accepted 16 October 2013
Available online 28 October 2013

Keywords:
Polycrystalline microstructure
Grain growth
Stress analysis
Monte Carlo simulation
Finite element method

ABSTRACT

A two-dimensional numerical model of microstructural effects is presented, with an aim to understand the mechanical performance in polycrystalline materials. The microstructural calculations are firstly carried out on a square lattice by means of a 2-D Monte Carlo (MC) simulation for grain growth, then the conventional finite element method is applied to perform stress analysis of a plane strain problem. The mean grain size and the average stress are calculated during the MC evolution. The simulation result shows that the mean grain size increases with the simulation time, which is about 3.2 at 100 Monte Carlo step (MCS), and about 13.5 at 5000 MCS. The stress distributions are heterogeneous in materials because of the existence of grains. The mechanical property of grain boundary significantly affects the average stress. As the grains grow, the average stress without grain boundary effect slightly decreases as the simulation time, while the one with strengthening effect significantly decreases, and the one with weakening effect increases. The average stress and the grain size agree well with the Hall–Petch relationship.

1. Introduction

Many materials, such as metallic alloys and ceramic composites used in engineering, have polycrystalline microstructures. It is well known that the material microstructure plays an important role in understanding the macroscopic response of real materials. The morphological characteristics of the materials, e.g., the size, shape, and orientation often govern their mechanical, physical, and chemical properties. A good understanding of the microstructure evolution during the preparation process such as sintering is required for optimizing the performance of the materials. The experimental methods for characterizing microstructure are usually achieved by means of scanning electron microscope (SEM) of the morphology of cross-section and fracture surface. However, the experimental measurements may consume a lot of time, and require high-resolution microscope equipments and high-quality material samples to characterize the microstructures.

During the last few decades, the researchers have made great progresses in modeling and simulating microstructure evolution using various computational approaches such as cellular-automaton [1–3], phase-field [4,5], and Monte Carlo (MC) [3,6,7] methods. The MC method is one of the most important methods owing to its simplicity and flexibility. Potts model was firstly employed to simulate the grain growth in two dimensions by Anderson and Srolovitz [8,9], and then many other researchers devoted to investigate the microstructure evolution of materials with single phase [6,10–12], two phases [13,14], or multiple phases [15], using MC or modified MC methods [3,16,17]. In addition, some mechanics can be quantificationally estimated by analyzing the field variables of materials undertaking loads using the finite element method (FEM). Guan and Geng [18] analyzed the stress distribution of a polycrystalline material with cavities on grain boundaries by FEM. Vedula et al. [19] predicted residual stresses and spontaneous microcracking upon cooling in polycrystalline alumina. Mori et al. [20] proposed a micro–macro method for simulating a sintering process of ceramic powder compacts based on the Monte Carlo and the finite element method. However, there is few systematic research on the effect of microstructure characteristics such as the size and number of grains on the stress response of the materials.

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http://dx.doi.org/10.1016/j.matdes.2013.10.047

The purpose of the present study is to investigate the mechanical performance of polycrystalline microstructures by combining the MC method and the finite element method. The remainder of this paper is organized as follows: Section 2 is devoted to a description of computational methods about Monte Carlo techniques and the finite element analysis. Section 3 gives the numerical results and discussion, and conclusions are summarized in Section 4.

2. Computational methods

2.1. Monte Carlo simulation

The application of the Monte Carlo technique to simulate grain growth has been described in detail [6,8,9,11,21], thus only the essential feature of this technique is addressed here. In the Monte Carlo approach the whole computational domain is discretised into a set of lattice grids, and a continuum microstructure is mapped onto the discretised domain. Each lattice grid, which belongs to a grain, is assigned with a random orientation number between 1 and Q, where Q is the total number of grain orientations. In this paper, the value of Q is 48. A grain is defined by a collection of grids that have the same orientation number. The grain boundary energy is specified by defining an interaction between nearest neighbor grids. Read and Shockley [22] derived an analytical expression $V(\theta)$ for the free energy of a low angle grain boundary to describe the grain boundary energy. $V(\theta)$ is given as follows:

$$V(\theta) = \begin{cases} J\frac{\theta'}{\theta^*}[1 - \ln(\frac{\theta'}{\theta^*})], & \theta' < \theta^* \\ J, & \theta \geqslant \theta^* \end{cases} \tag{1}$$

where J is a positive constant which sets the scale of the grain boundary energy, $\theta' = \begin{cases} |\theta|, & 0 \leqslant |\theta| \leqslant \pi \\ 2\pi - |\theta|, & \pi \leqslant |\theta| \leqslant 2\pi \end{cases}$. θ^* is the value of misorientation parameter, θ, above which grain boundaries are considered to be high angle.

The local interaction energy, E_{loc}, as a function of the grain misorientation across the boundary is calculated by the Hamiltonian which sums the interfacial energy of the neighbor grids:

$$E_{loc} = \sum_{j=1}^{n} V(\theta)(1 - \delta_{S_i S_j}) \tag{2}$$

where $\theta = 2\pi(S_i - S_j)/Q$, δ is the Kronecker's delta function, S_i the orientation of lattice grid i, S_j represents the orientations of its nearest neighbors, and n the total number of the nearest neighbor grids.

The kinetics of the grain boundary migration are simulated by judging the change of attempted orientation based on the energy change, and the probability of orientation change is defined as:

$$P = \begin{cases} 1, & \Delta E \leqslant 0 \\ \exp(-\Delta E/k_B T), & \Delta E > 0 \end{cases} \tag{3}$$

where ΔE is the change of energy, k_B the Boltzmann constant, and T the temperature.

2.2. Monte Carlo algorithm

A 2-D problem is considered for the sake of simplicity. An iterative procedure applied to perform the grain growth is given as follows:

(1) Generate a two dimensional $N_1 \times N_2$ lattice grids as mentioned above, where N_1, N_2 are numbers of the discretised lattice points in two directions.
(2) Assign each of the lattice grids a random orientation number termed as S_i.
(3) Select a trial grid (ix, iy) in the lattice and note its orientation as S_{iold}.
(4) Find the neighbors of the selected grid.
(5) Calculate local interaction energy (E_{loc1}) before reorientation by Eq. (2).
(6) Generate randomly a new trial orientation number of the selected grid, and note it as S_{inew}.
(7) Calculate local interaction energy (E_{loc2}) at the new trial orientation state by Eq. (2).
(8) Calculate the energy change (ΔE) between E_{loc1} and E_{loc2}.
(9) Calculate the probability of orientation change by Eq. (3) to judge the reorientation. If $\Delta E \leq 0$, accept the reorientation, and change the initial orientation (S_{iold}) to attempted orientation (S_{inew}). If $\Delta E > 0$, then generate a random number p between 0 and 1, if $P \geqslant p$, accept the reorientation, restore the orientation otherwise. Repeating (3–9) steps for all the lattice grids to finish a Monte Carlo step (MCS), corresponding to $N_1 \times N_2$ reorientation attempts. The simulation time is measured in terms of MCS. The above steps are repeated until the desired step number is reached.

2.3. Finite element analysis

2.3.1. Basic equation

In the numerical computation of mechanical behaviors of polycrystalline materials, we apply fundamental equations of elasticity theory including equilibrium equations, kinematics equations, and constitutive equations.

Consider a body $\Omega \subset R^2$ with boundary Γ. The equilibrium equations and boundary conditions are given by

$$\begin{aligned} &\nabla \cdot \sigma + b = 0, \text{in } \Omega \\ &u = \bar{u}, \text{on } \Gamma_u \\ &\sigma \cdot n = \bar{t}, \text{on } \Gamma_t \end{aligned} \tag{4}$$

where n is the unit outward normal, σ the Cauchy stress, and b the body force per unit volume. The kinematics equations consist of the strain–displacement relation

$$\varepsilon = \varepsilon(u) = \nabla_\varepsilon u \tag{5}$$

where ∇_ε is the symmetric part of the gradient operator. The constitutive relation is given by Hooke's law.

$$\sigma = C : \varepsilon \tag{6}$$

where C is the Hooke's elasticity tensor.

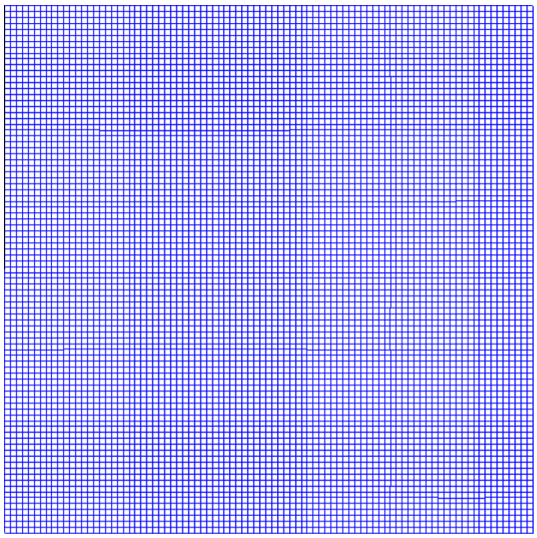

Fig. 1. Mesh.