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

Yunfang Liu [a], Laifei Cheng [a], Qingfeng Zeng [a,*], Zhiqiang Feng [b,c,*], Jin Zhang [a], Junhui Peng [a], Congwei Xie [a], Kang Guan [a]

[a] Science and Technology on Thermostructural Composite Materials Laboratory, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, People's Republic of China
[b] School of Mechanics and Engineering, Southwest Jiaotong University, Chengdu, Sichuan 610031, People's Republic of China
[c] Laboratoire de Mécanique et d'Energétique, Université d'Evry, Evry 91020, France

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.

© 2013 Elsevier Ltd. All rights reserved.

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.

* Corresponding authors. Addresses: School of Materials Science & Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, China (Q. Zeng), School of Mechanics & Engineering, Southwest Jiaotong University, Chengdu, Sichuan 610031, China (Z. Feng). Tel.: +86 29 88495619; fax: +86 29 88494620.
E-mail addresses: qfzeng@nwpu.edu.cn (Q. Zeng), feng@ufrst.univ-evry.fr (Z. Feng).

0261-3069/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
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.

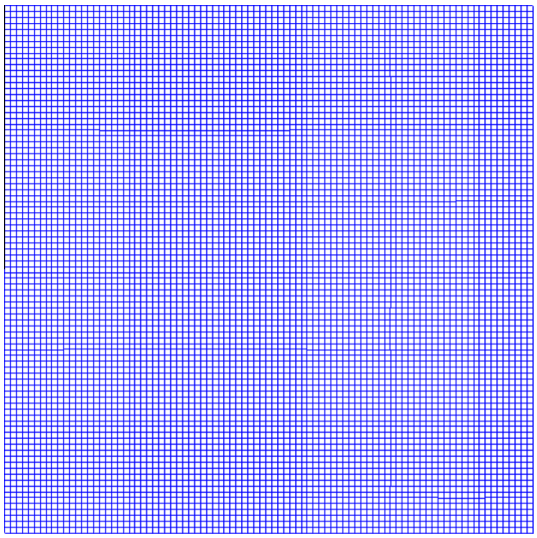

Fig. 1. Mesh.

2.3.2. Computational model

We assume that a cross-section of a material is taken into account, and a plane strain problem neglecting body forces is considered here. The 2D finite element model corresponding to the microstructure is utilized for the numerical mechanical analysis. The material is assumed to be linearly elastic. The geometry parameters are the total width $L = 0.01$ m, and the total height $H = 0.01$ m. The left boundary is assigned to be symmetrical boundary, the top and bottom boundary are free, and a given displacement $u = 2e - 3L$ is applied to the right boundary of the geometry model. The 4-node element is used in the analysis, and the nodes correspond to the grids obtained by the MC technique. Fig. 1 shows the mesh of the model.

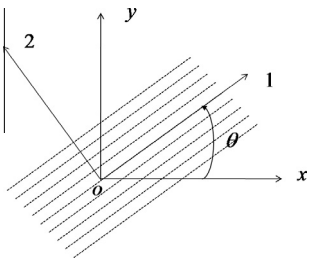

Fig. 2. Grain orientation.

Table 1
Parameters for Monte Carlo simulation.

Interface energy (J/m^2)	1 [12]
Temperature (K)	1773
Misorientation parameter	0.3π [24]
Boltzmann constant (J/K)	1.38e−23

2.3.3. Material properties

Let *xoy* be a fixed coordinate system, and the grain orientation θ is shown in Fig. 2. $E = 300$ GPa, $v = 0.21$ are the Young's modulus and Poisson ratio, respectively. D is the elasticity matrix, which will be transformed by taking into account the grain orientation. The transformation equation is listed as follows:

$$T = \begin{bmatrix} \cos^2\theta & \sin^2\theta & 2\sin\theta\cos\theta \\ \sin^2\theta & \cos^2\theta & -2\sin\theta\cos\theta \\ -\sin\theta\cos\theta & \sin\theta\cos\theta & \cos^2\theta - \sin^2\theta \end{bmatrix} \quad (7)$$

3. Numerical results and discussion

In this work, several numerical tests are carried out to investigate the effect of the microstructure on the mechanical performance. The procedures of obtaining the microstructure have been implemented by Matlab code, while the finite element analysis procedures have been implemented in C++, and the results are displayed by the postprocessing software FERView [23].

3.1. Grain orientation and stress distribution

The parameters used in the simulation are given in Table 1.

For convenient calculation, the positive constant J is set to 1 [12]. A sintering temperature is selected to the simulation temperature. Yu and Esche [24] has studied the effect of the parameter $\theta^*(\theta^* = 0, 0.3\pi, 0.6\pi, \pi)$ on the grain growth kinetics, and pointed out that the mean values of the grain growth exponent remain essentially unchanged with θ^* varying from 0 to π, and here θ^* is set to 0.3π.

Fig. 3 shows the microstructure evolution obtained by Monte Carlo techniques. It is over six times periods, ranging from time $t = 0$ MCS to $t = 5000$ MCS. As it is shown, the initial grain states are of a random distribution occupying 100×100 grids. It was confirmed by the detailed examination of the simulated microstructures that some grains shrink and ultimately disappear, some

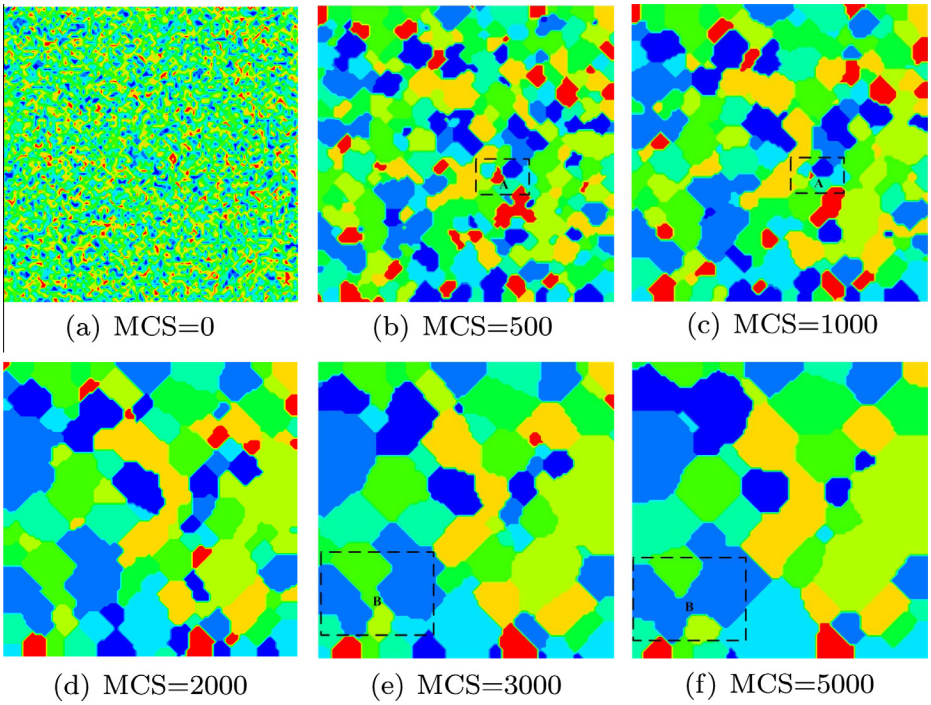

Fig. 3. The microstructure evolution obtained by Monte Carlo techniques.

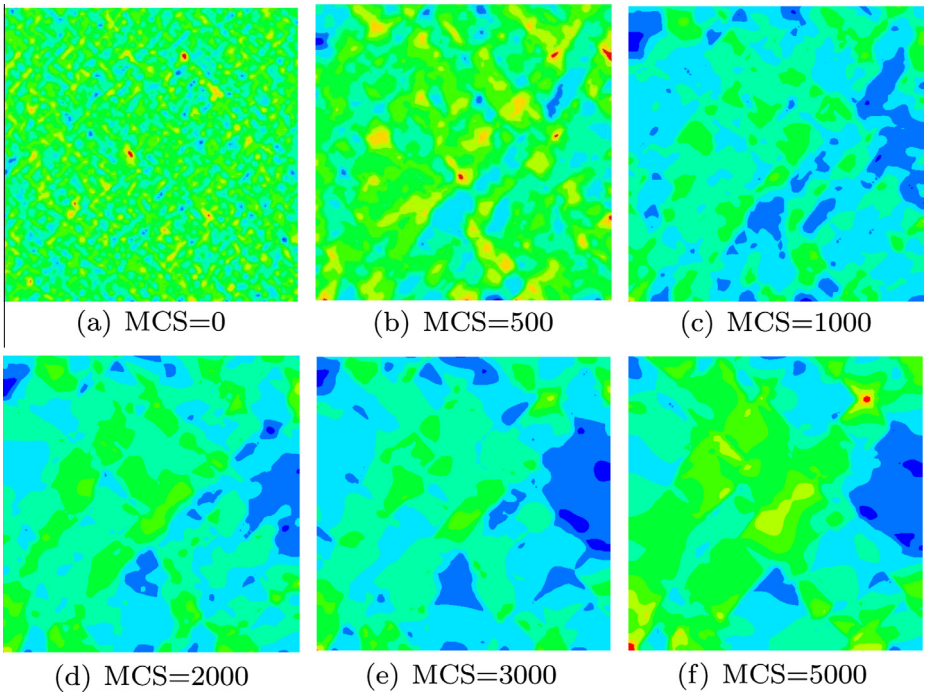

Fig. 4. Stress distribution along x direction.

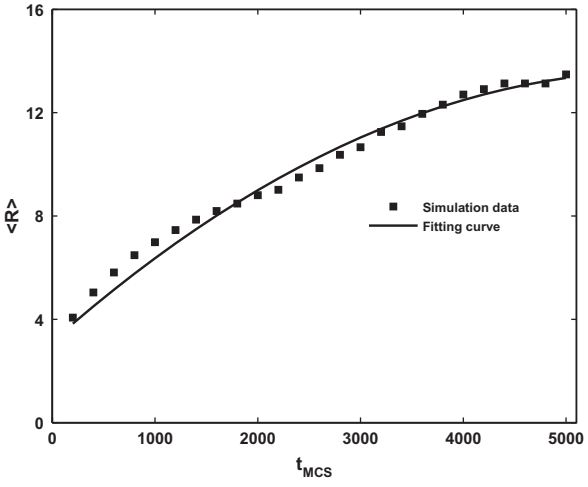

Fig. 5. Mean grain size $\langle R \rangle$ vs. simulation time t_{MCS}.

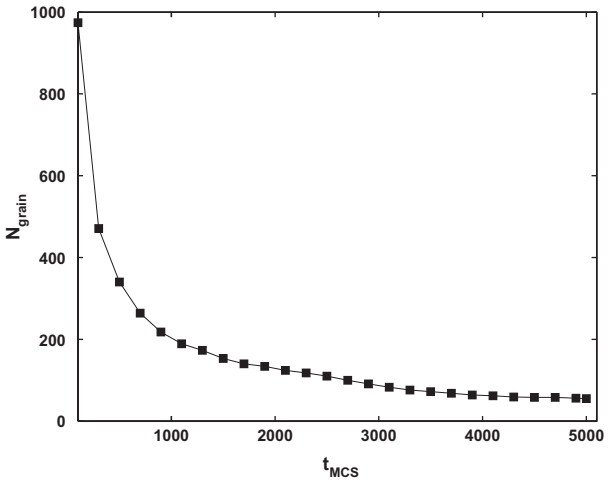

Fig. 6. Number of grains N_{grain} vs. simulation time t_{MCS}.

grains grow up at the early stage, but shrink at the later stage, and some grains continue to grow (see the grains marked by A). In addition, it can be observed that grain rotation coalescence are happened in some cases during the evolution as indicated previously [7,25]. Two small grains with the same orientation which are not adjacent to each other, grow up by swallowing the grain between them to make the grain boundaries migrate close to each other, and, finally, combine into a large one (see the grains marked by B).

Fig. 4 shows the x stress of the microstructure effect. It is obvious that the stress distributions are heterogeneous due to the presence of the grains with different orientations, which coincides with the conclusion that the stress distribution pattern is affected by the orientations of the grains [18]. From the contours in Figs. 3 and 4, it is evident that the outline of stress is affected by the grain shape, and the material non-homogeneity significantly alters the stress distribution. The stress distribution profile changes as the microstructure changes through out the whole MCS.

3.2. The mean grain size, the number of grains and the average stress

To view the simulation results quantitatively, the mean grain size, the number of grains, and the average stress are calculated. The grain area, A, is the number of lattice grids within one grain. The grain size, R, is usually defined as the square root of the grain area [12]. The mean grain size, $\langle R \rangle$, is defined as the square root of the total number of lattice grids divided by the total number of grains, and the average stress, $\langle \sigma \rangle$, is defined as the average volume stress.

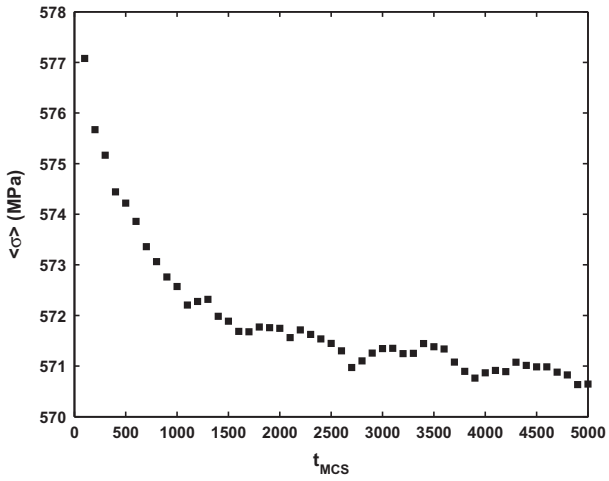

Fig. 7. Average stress along x direction $\langle\sigma\rangle$ vs. simulation time t_{MCS}.

$$\langle R\rangle = \sqrt{\frac{N}{N_{grain}}} \tag{8}$$

$$\langle\sigma\rangle = \frac{1}{V}\int_{\Omega}\sigma dV \tag{9}$$

where, N is the total number of lattice grids, N_{grain} is the number of grains of the microstructure, V is the volume of the domain Ω.

The plots of the mean grain size versus the simulation time is shown in Fig. 5. The mean grain size increases continuously with the simulation time, which is about 3.2 at 100 MCS, and increases to 13.5 at 5000 MCS.

Fig. 6 depicts the evolutions of the number of grains as a function of the Monte Carlo steps in the above simulation. The number of grains is found to decrease with the simulation time, which is about 974 at 100 MCS, as indicated, and after 5000 MCS only about 55 remains. The number of grains decreases fast at the early stage (MCS < 1000), while the decrease is slow at the later stage (MCS > 1000). The grains grow in a long time, but the structure is still polycrystalline with finite grains. As expected, the polycrystalline microstructures are hard to transform into a single grain structure.

Fig. 7 shows the average stress along x direction versus simulation time. It can be seen that the average stress in the material slightly decreases as the simulation time increases, from about 577 MPa (MCS = 100) to about 571 MPa (MCS = 5000).

3.3. The effect of grain boundary on the stress

The effect of grain boundary was not considered in the results obtained above, which actually plays an important role in the mechanical performance of the microstructure, such as strengthen or weaken effect. In this subsection, we introduce a grain boundary between two grains, and assign it to be another material with Young's modulus E_2. To be specific, it composes of the elements whose nodes have different orientations. The microstructure with grain boundary is shown in Fig. 8(a). The effect of grain boundary

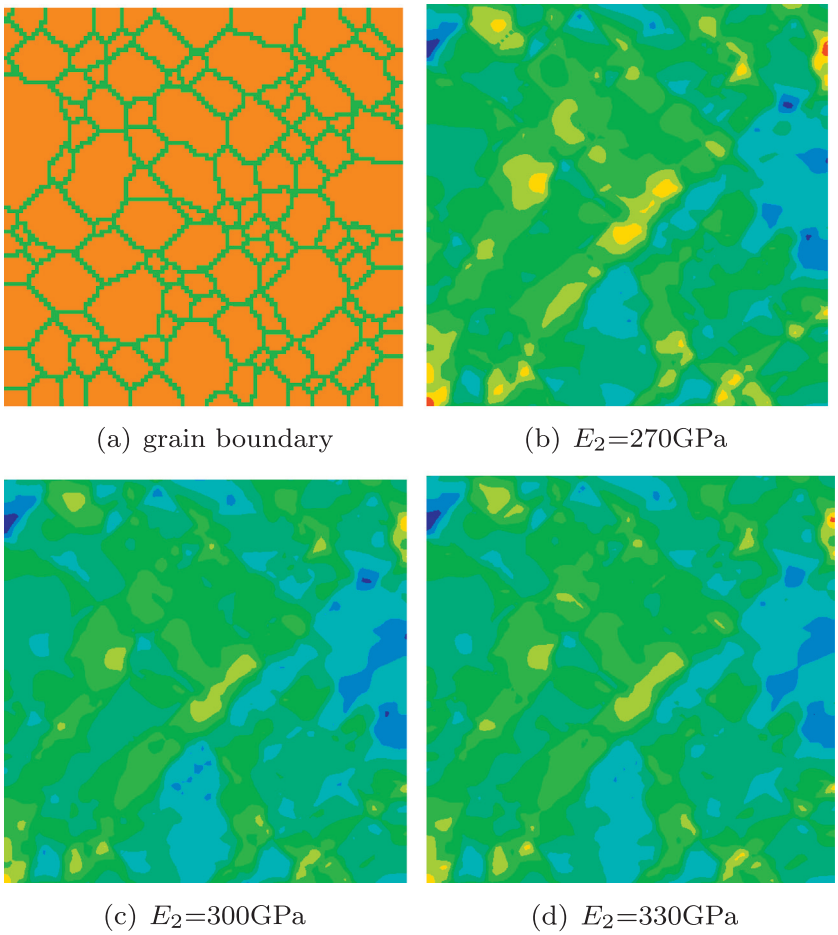

Fig. 8. Microstructure with grain boundary and the stress distribution along x direction.

on the stress is investigated with results of several cases shown in Fig. 8(b–d). E_2 = 270, 300, 330 GPa are for the cases that with weaken effect, without boundary effect, and with strengthen effect, respectively. Note that the general outline of the stress does not change obviously, but the magnitudes of that are different from each other, which is easily recognized from the contour colour.

The macro-mechanical properties of grain scale microstructure depend on a variety of factors including components, structure characters such as the grain size and grain boundary. Fig. 9 shows the average stress along x direction versus the grain size for five cases with different E_2, suggesting that, in a given MCS state (a given grain size), the larger the modulus of the grain boundary (E_2) is, the larger the stress is. It can also be seen that the average stress in the material without grain boundary effect (E_2 = 300 GPa) slightly decreases as the simulation time increases, while the stresses of the other four cases with grain boundary effect change significantly. The stress in the structures which are strengthened by the grain boundary effect (E_2 = 330, 360 GPa) distributes in the upper side of the first case, and decreases as the grains grow, while it increases in the structures which are weakened by the grain boundary effect (E_2 = 240, 270 GPa).It could be explained with the fact that the grain boundary effect decreases with the increases of grain size. We replot the data, and find that the average stress proportionally increases to the minus square foot of the mean grain size (Fig. 10). The average stress and the grain size obtained agree well with the Hall–Petch relationship $\sigma = \sigma_0 + kR^{-\frac{1}{2}}$ [26], which is established for polycrystalline materials based on experimental data by Hall [27] and Petch [28], and is widely applied for experimental study [29].

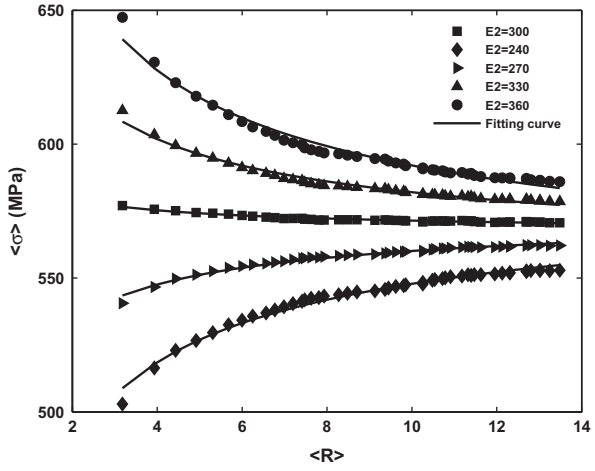

Fig. 9. Average stress along x direction $\langle\sigma\rangle$ vs. mean grain size $\langle R\rangle$.

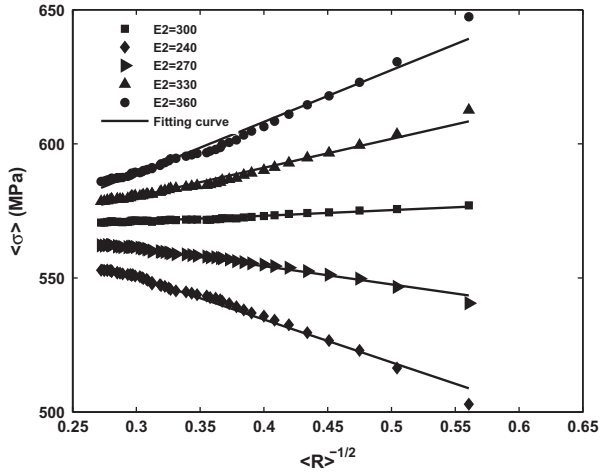

Fig. 10. Average stress along x direction $\langle\sigma\rangle$ vs. mean grain size $\langle R\rangle^{-1/2}$.

4. Conclusions

A microstructure-based finite element method has been presented for two-dimensional mechanical analysis. The microstructure evolution and the stress distribution have been analyzed by discussing the number of grains, the mean grain size, and the average stress of the polycrystalline microstructures. The mean grain size increases continuously with simulation time, while the number of grains decreases with simulation time. The mean grain size is about 3.2 at 100 MCS, and increases to 13.5 at 5000 MCS. The number of grains at 100 MCS is about 974, after 5000 MCS only about 55 remains. The stress distributions are heterogeneous in the structure because of the existence of the 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 decreases, and the one with weakening effect increases. The average stress and the grain size agree well with the Hall–Petch relationship.

Acknowledgements

This work is supported by the Research Fund of the State Key Laboratory of Solidification Processing (No. 65-TP-2011), Foreign Talents Introduction and Academic Exchange Program (No. B08040), National Natural Science Foundation of China (No. 51372203), and the Basic Research Foundation of NWPU (No. JCY20130114).

References

[1] Geiger J, Roósz A, Barkóczy P. Simulation of grain coarsening in two dimensions by cellular-automaton. Acta Mater 2001;49:623–9.
[2] Raghavan S, Sahay SS. Modeling the grain growth kinetics by cellular automaton. Mater Sci Eng A 2007;445–446:203–9.
[3] Sieradzki L, Madej L. A perceptive comparison of the cellular automata and Monte Carlo techniques in application to static recrystallization modeling in polycrystalline materials. Comput Mater Sci 2013;67:156–73.
[4] Krill III CE, Chen LQ. Computer simulation of 3-D grain growth using a phase-field model. Acta Mater 2002;50:3057–73.
[5] Wang YU. Computer modeling and simulation of solid-state sintering: a phase field approach. Acta Mater 2006;54:953–61.
[6] Blikstein P, Tschiptschin AP. Monte Carlo simulation of grain growth. Mater Res 1999;2:133–7.
[7] Hafez Haghighat S, Karimi Taheri A. An analytical and experimental investigation on the normal grain growth in metals using the Monte Carlo method. Mater Des 2007;28:2533–9.
[8] Anderson M, Srolovitz D, Grest G, Sahni P. Computer simulation of grain growth–I. Kinetics. Acta Metall 1984;32:783–91.
[9] Srolovitz D, Anderson M, Sahni P, Grest G. Computer simulation of grain growth–II. Grain size distribution, topology, and local dynamics. Acta Metall 1984;32:793–802.
[10] Allen J, Cornwell C, Devine B, Welch C. Simulations of anisotropic grain growth in single phase materials using Q-state Monte Carlo. Comput Mater Sci 2013;71:25–32.
[11] Srolovitz D, Grest G, Anderson M. Computer simulation of grain growth–V. Abnormal grain growth. Acta Metall 1985;33:2233–47.
[12] Yu Q, Nosonovsky M, Esche SK. Monte Carlo simulation of grain growth of single-phase systems with anisotropic boundary energies. Int J Mech Sci 2009;51:434–42.
[13] Cheng H, Huang C, Liu H, Zou B. Monte Carlo simulation of microstructure evolution in nano-composite ceramic tool materials. Comput Mater Sci 2009;47:326–31.
[14] Fang B, Huang C, Liu H, Xu C, Sun S. Monte Carlo simulation of grain-microstructure evolution in two-phase ceramic tool materials. J Mater Process Technol 2009;209:4568–72.

[15] Hao S, Huang C, Zou B, Wang J, Liu H, Zhu H. Three dimensional simulation of microstructure evolution for ceramic tool materials. Computer Mater Sci 2011;50:3334–41.
[16] Esche SK. Monte Carlo simulations of grain growth in metals. In: Mordechai S, editor. Applications of Monte Carlo method in science and engineering: InTech; 2011. p. 581–610.
[17] Yu Q, Esche SK. A Monte Carlo algorithm for single phase normal grain growth with improved accuracy and efficiency. Comput Mater Sci 2003;27:259–70.
[18] Guan X, Geng XL. Stress distribution near cavity on grain boundary. J Northwestern Polytech Univ 2004;22:726–9.
[19] Vedula VR, Glass SJ, Saylor DM, Rohrer GS, Carter WC, Langer SA, et al. Residual-stress predictions in polycrystalline alumina. J Am Ceram Soc 2001;84:2947–54.
[20] Mori K, Matsubara H, Noguchi N. Micro–macro simulation of sintering process by coupling Monte Carlo and finite element methods. Int J Mech Sci 2004;46:841–54.
[21] Grest G, Srolovitz D, Anderson M. Computer simulation of grain growth–IV. Anisotropic grain boundary energies. Acta Metall 1985;33:509–20.
[22] Read W, Shockley W. Dislocation models of crystal grain boundaries. Phys Rev 1950;78:275–89.
[23] Feng ZQ, Feng ZG. FER/view: an interactive finite element post-processor. In: Yao ZH, Yuan MW, Zhong WX, editors. Computational mechanics. WCCM VI in conjunction with APCOM04; Beijing, China: Springer; 2004.
[24] Yu Q, Esche SK. Modeling of grain growth kinetics with Read–Shockley grain boundary energy by a modified Monte Carlo algorithm. Mater Lett 2002;56:47–52.
[25] Moldovan D, Wolf D, Phillpot SR, Haslam AJ. Role of grain rotation during grain growth in a columnar microstructure by mesoscale simulation. Acta Mater 2002;50:3397–414.
[26] Hansen N, Ralph B. The strain and grain size dependence of the flow stress of copper. Acta Metall 1982;30:411–7.
[27] Hall EO. The deformation and ageing of mild steel: III Discussion of results. Proc Phys Soc B 1951;64:747–53.
[28] Petch N. The cleavage strength of polycrystals. J Iron Steel Inst 1953;174:25–8.
[29] Fu MW, Chan WL. Geometry and grain size effects on the fracture behavior of sheet metal in micro-scale plastic deformation. Mater Des 2011;32:4738–46.