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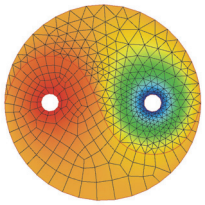

SIMULATION OF DYNAMIC RECRYSTALLIZATION USING RANDOM GRID CELLULAR AUTOMATA

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Abstract

Computer simulation is a powerful tool to predict microstructure and its evolution during dynamic recrystallization. Cellular Automata (CA), as one of the most efficient approaches proposed to simulate physical models of recrystallization and grain growth. In this study, the recrystallization and growth phenomena were modelled using a two dimensional random-grid CA method. Time, initial grain size and initial nuclei density as Johnson, Mehl, Avrami, and Kolmogorov (JMAK) variables have been used to validate the current model. Considering the model assumptions, it is shown that the CA can successfully simulate dynamic recrystallization.

Key words: dynamic recrystallization, dislocation density, cellular automata

1. INTRODUCTION

Recrystallization, the formation of new strain-free grains in certain parts of the specimen and the subsequent growth of these grains to consume the deformed or recovered microstructure, has been simulated by a number of approaches to predict the final microstructure. These approaches have been simply modelled using the JMAK theory (Humphreys & Hatherly, 1996). In real materials, the ideal JMAK behaviour is rarely observed because of the heterogeneous nature of nucleation and growth. However, the (CA) model gives a time and space dependent description of the recrystallization. As a numerical approach, CA provides a virtual visible evolution of the microstructure during recrystallization.

In CA, the domain is divided into cells; each of them has a defined state. This state refers to the grain to which the cell belongs (Raabe, 1998). CA computes the evolved microstructure by updating the state of all cells; the new state depends on the state of cells in a defined neighbourhood. In conventional CA, an equi-distant grid is used to distribute the cells (Raabe, 2002). While the early work used a regular cell arrangement, recent developments (Raabe 1998) have allowed the use of a random grid. The concept of the spatial resolution of cellular automata can be defined as the number of cells per unit area. According to spatial resolution definition, conventional CA has a constant resolution, whereas it varies in random CA (figure 1). Each cell in the simulation scale is given a specific digit which represents the orientation of each grain and will not change during simulation. The cells which have the same digits belong to the same grain and grain boundaries are determined according to the neighbouring cells of adjacent grains with different digits.

In this study, random cellular automaton on a two dimensional grid with a periodic boundary condition are used. The initial nuclei density and neighbourhood radius have been entered to the model as primary variables. The cells are dispersed

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uniformly and there was no preference between cells to be a nucleus. Therefore, the simulated results can be compared with ideal JMAK theory which shows a good agreement with the homogenous recrystallization result. Then, heterogeneous recrystallization is considered and dislocations are distributed on the domain according to stress-strain curve derived from a hot torsion test. When the critical dislocation density, ρ_{cr}, is exceeded in a cell, the cell will change its state from an unrecrystallized cell to the recrystallized (RX) cell. The model is verified by comparing the simulation results of the dislocation density-time curve with experiments in terms of final size of the grains in the domain.

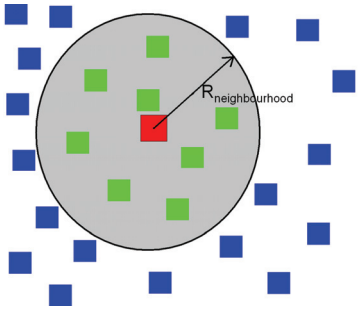

Fig. 1. *Neighbourhood definitions in random grid cellular automata (Raabe 2002).*

2. FORMULATION OF THE CA MODEL

In the current model, an initial domain of 100 × 100 cells was used to reduce the running time and memory usage. The first neighbourhood radius was defined to be 3, but it can be changed as one of the initial variables. To obtain the original microstructure a parameter is identified to determine the initial grain size. In this model, it is assumed that all the cells are identical; therefore, the critical dislocation density is equal to the critical dislocation density of each cell. In the initial microstructure, each grain is distinguished by two parameters; firstly, its own digit which represents its orientation and shows a specific colour and secondly a grain boundary which is distinguished by one layer of cells. By measuring the critical stress from experimental results and calculating the consequent critical dislocation density, ρ_{cr}, the model can simulate recrystallization. The stages of simulation are as following:

1 - An initial microstructure with an initial average grain size is introduced.

2 - The dislocation difference in each time step ($\Delta\rho/\Delta t$) is computed from the ρ-t curve (figure 2) which is obtained from experimental stress-strain results by the equation:

$$\sigma = \sigma_0 + \alpha G b \sqrt{\rho} \qquad (1)$$

where, α is a dislocation interaction term and is constant for most metals (Hodgson, 1993), G is the shear modulus (Pa)(Roucoules & Pietrzyk, 2003) and b is the Burgers vector (Hodgson, 1993).

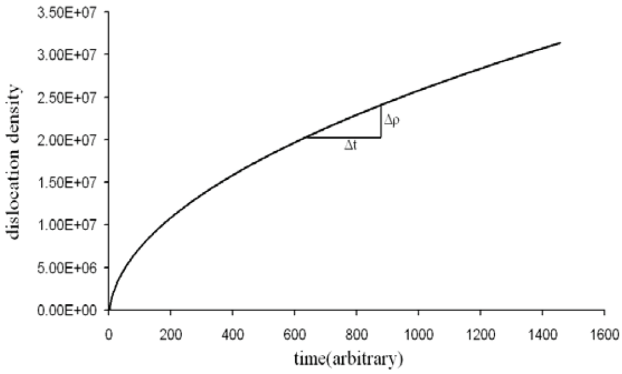

Fig. 2. *calculating dislocation difference in each time step.*

3 - This increment of dislocation density (Δρ) is randomly dispersed over the domain.

4 - Dislocations migrate among cells when the transition rules are satisfied (transition rules of migration are explained in the following).

5 - Dislocations accumulate and reach the critical density (which was calculated from the critical stress).

6 - Nucleation happens in the cells in which the dislocation density has reached the critical density.

According to the literature (Raabe, 2002), nucleation of new grains takes place near grain boundaries. Therefore, the model reflects this by proper transition rules. By assuming that dislocations of cell A will migrate to cell B (figure 3.a), the transition rules of migration are summarized as following:

a) Cell B is not located on any of the surrounding grain boundaries.

b) Cell B is the neighbourhood of cell A (according to defined neighbourhood radius) (figure 3.a).

c) Cell B is in the same grain as cell A (figure 3.b).

d) The total dislocations in cell B are lower than in cell A.

Dislocations migrate from one cell to adjacent cells that belong to the same grain. However, they cannot cross the grain boundaries. This leads to an increase in the dislocation density near the grain boundaries and triple junctions. It should be noted that triple junctions are more preferable locations for recrystallization than grain boundaries (Raabe, 2002), which has also been demonstrated in the current model (figure 3.b).

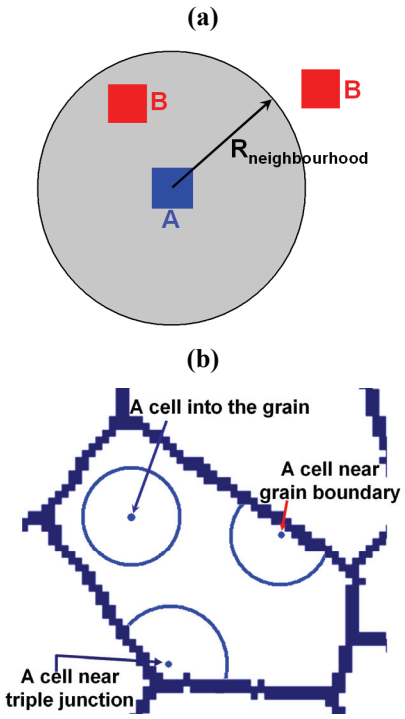

Fig. 3. Neighbourhood definition (a), three cells in different positions in microstructure (b).

As illustrated in figure 3.b, by considering an individual cell in the domain, the number of dislocations increases near grain boundaries and triple junctions. So, there is a dislocation gradient between the centre and the boundary of each grain. For the same reason and considering that triple junctions have higher defect energy than grain boundaries, a large number of dislocations accumulate at these points (figure 4.b). Therefore, they reach the critical value for a nucleus formed earlier.

3. JMAK VALIDATION OF BASIC CA MODEL FOR STATIC RECRYSTALLIZATION

As explained earlier, in the first section of simulation, homogeneous recrystallization is modelled in which the initial nuclei have been nucleated in the microstructure regardless of the cell position; that is, there is no preference between cells to nucleate. To verify the CA model, the simulation results are compared with the ideal JMAK theory. The result obtained from the CA model shows that the mean grain size is the most frequent (i.e. the mode) size in homogeneous microstructure, which is in good agreement with the ideal JMAK theory (figure 5).

The main point is that the grain size frequency is independent of the initial nuclei size i.e. the initial grain size does not affect the output. However, the final grain size does depend on the initial nuclei density and the higher the initial nuclei density, the earlier the grains will impinge on each other and the microstructure will exhibit a more uniform grain size (figure 5.b). In the latter condition, the deviation from the mean grain size is smaller than for a low nuclei density. Therefore, the initial nuclei density is the main parameter which controls the final grain size. Figure 6 shows the Avrami plot to determine the exponent, n, which has a value of 3.0 for site-saturated conditions. The simulations with a very high initial density of nuclei reveal a more pronounced deviation from the straight line during the beginning of recrystallization. The plot is generally linear with time until impingement and is largely independent of nuclei density. In the Avrami plot the straight lines depend on the nucleation rate. By measuring the recrystallized volume fraction in different time steps, it is indicated that all graphs are linear with the slope between 2 and 3 which is in a good agreement with linear Avrami plot (figure 6).

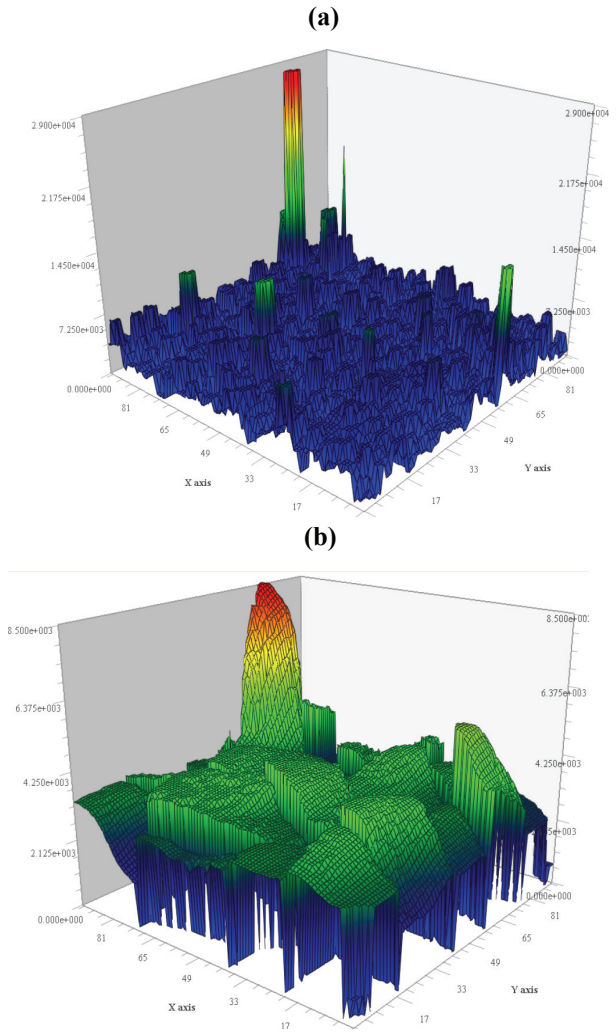

Fig. 4. Dislocations increase on each grain during deformation. Dislocation gradient is indicated in each grain.

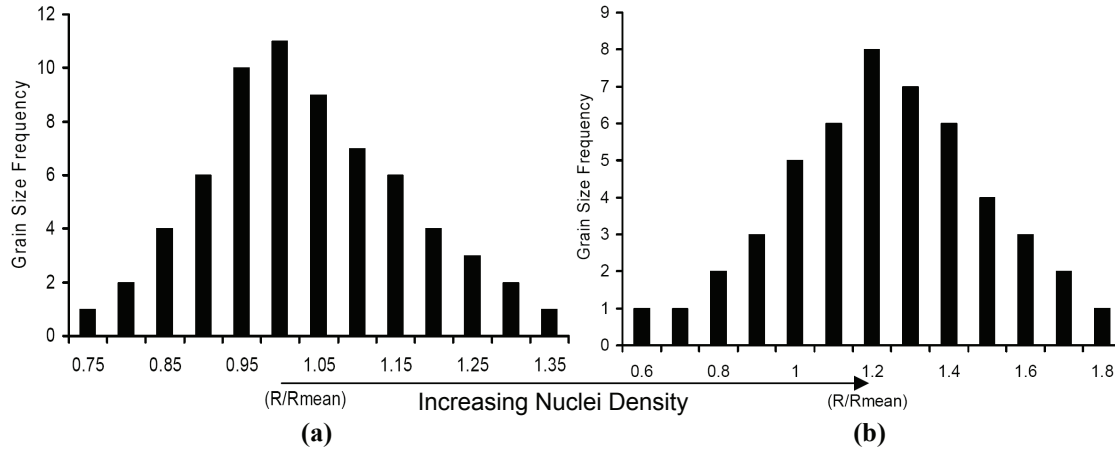

Fig. 5. Grain size frequency in Avrami plot according to simulation results, (a) low initial nuclei density,(b) high initial nuclei density.

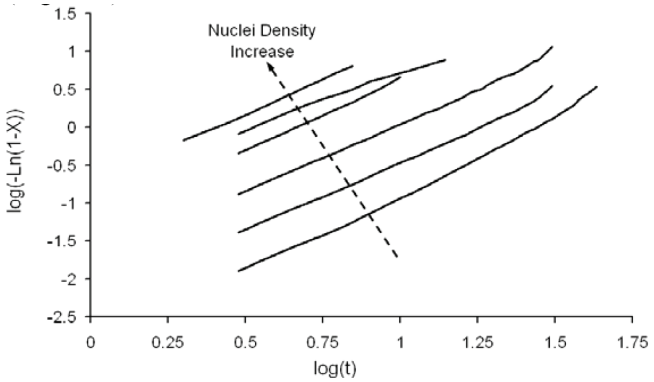

Fig. 6. Avrami plot obtained from simulation.

elsewhere (Hodgson, 1993). A roughing process at 1200°C was used to achieve an initial homogenized microstructure with an average grain size about 20 μm (figure 7.a) and 35 μm (figure 7.b). The samples were then cooled at 1°C / s at 900 °C, held for 2 min and deformed at strain rate of 0.01 s^{-1}. Then, the samples were quenched immediately (<0.5 s) after deformation (figure 7a,b).

The stress-strain curves obtained from the experimental results are shown in figure 8. As can been seen, by increasing the strain the stress will increase in the material up to a critical stress at

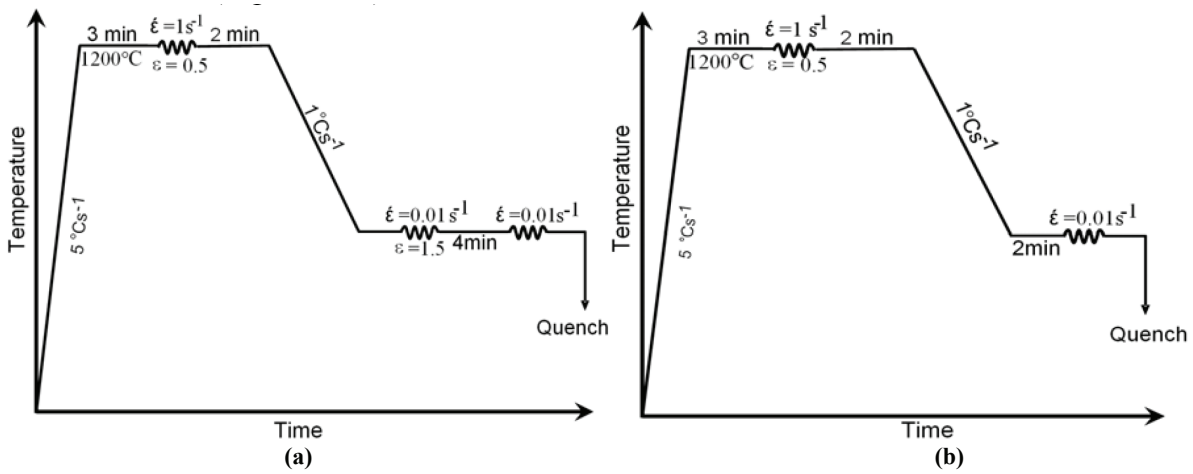

Fig. 7. Programme of hot torsion test used in the study (a) d_0=20 μm, (b) d_0=35 μm.

4. EXPERIMENTS

The experimental data was generated as a part of another project by Dehghan et al.(2004). 304 austenitic stainless steel with a chemical composition (wt%) of Fe-0.02%C-1.6%Mn-8.2%Ni-18.5%Cr-0.8%Cu was used in this study. Torsion samples with a gage length of 20 mm and a diameter of 6.7 mm were machined from the rolled billets. The torsion equipment used in this study has been described

which dynamic recrystallization initiates followed by a work softening process.

Under these conditions, a critical dislocation density (ρ_{cr}) is reached which can be estimated by using the critical stress. To measure the critical stress, the work hardening rate ($\theta=d\sigma/d\varepsilon$) versus stress ($\sigma$) was drawn (figure 9.a) and has been used in earlier studies (Militzer & Jonas, 1994; Mecking & Kocks, 1981; Poliak & Jonas, 2003). It was shown by Poliak and Jonas (2003) that an inflection

point on the work hardening curve represents the initiation of dynamic recrystallization (figure 9.b).

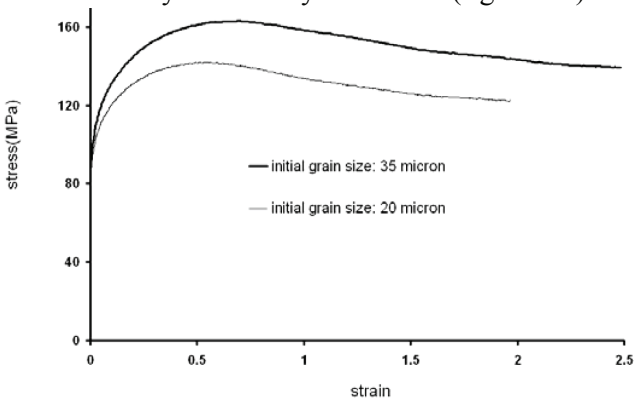

Fig. 8. *Stress-strain curve obtained from experimental results (T=900 °C, $\dot{\varepsilon} = 0.01\ s^{-1}$).*

stress and the peak stress, the dislocation difference ($\Delta\rho=\rho_2-\rho_1$) is positive i.e. the rate of dislocation generation (ρ_2) is higher than that of dislocation annihilation (ρ_1). Dislocations were generated through deformation and annihilated when new nuclei nucleated (Mecking, 1981). Due to the latter phenomenon, the dislocation level of the recrystallized nuclei decreased to the reference level. After the peak stress, $\Delta\rho$ is negative. This means that the rate of dislocation generation is lower than that of dislocation annihilation. To calculate the number of dislocations generated during deformation after peak stress, the dislocations removed by both recrystallizing new nuclei and growing recrystallized grains should firstly be computed. The difference between

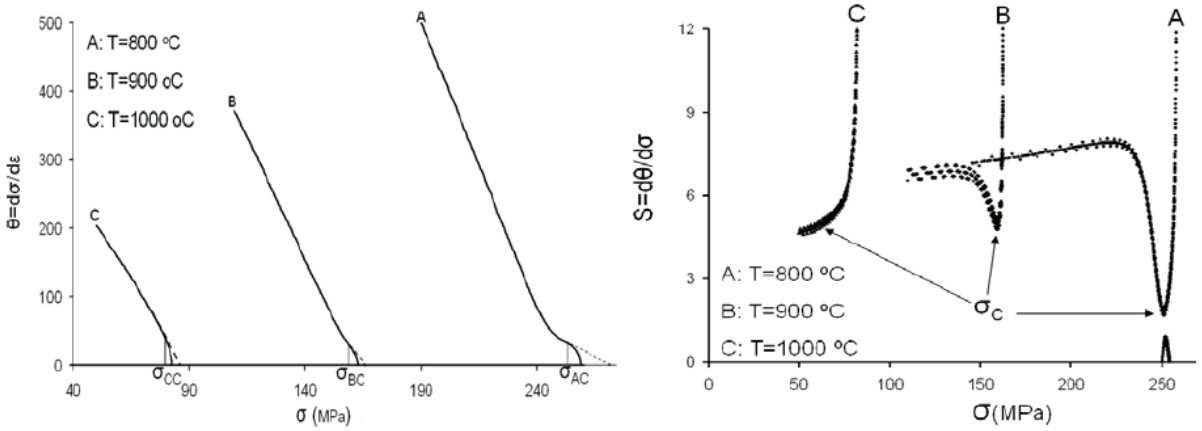

Fig. 9. *Determining critical dislocation density through (ρ-t) curve.*

If the dislocation amount of each cell reaches the critical value, the cell changes its state from an unrecrystallized cell to a recrystallized one and its dislocation density decreases to the reference value. So, there is a dislocation density difference ($\Delta\rho$) between a recovered and a recrystallized grain which is equal to the number of dislocations removed by the generation of new recrystallized grains. In the model, the dislocations were distributed uniformly over all cells at the first time increment according to dislocation theory (Estrin & Mecking, 1984) (figure 10). In the following time steps, dislocations were distributed randomly throughout the model by calculating the generated dislocations as a result of deformation which was determined from the ρ-t curve. Grain boundaries are considered as dislocation sinks. Therefore, the dislocation density at the grain boundaries was set to the reference value (figure 10.a).

After exceeding the critical dislocation density, deformation and recrystallization happen simultaneously in the domain. However, between the critical removed dislocations (ρ_1) and the dislocation difference ($\Delta\rho$) is the number of dislocations generated by deformation. A dislocation density increment ($\Delta\rho$ in figure 2) is dispersed on the domain in each time step. After nucleation, the nuclei grow until they impinge on each other, finally resulting in a fully recrystallized microstructure. At the end, several parameters can be extracted from the model, including final size and dislocation density of each grain and average grain size, recrystallized volume fraction, stress and strain of the domain.

The model was validated by comparing simulated results with the experimental results in terms of final grain size. Two microstructures with different initial grain size have been considered to compare the experimental and simulated results. The results taken from dislocation density-time step curves have a good agreement with the results driven from simulation for two different initial grain sizes (figure 11). Regardless of the initial grain size, the simulated curve under-estimates the results of torsion test.

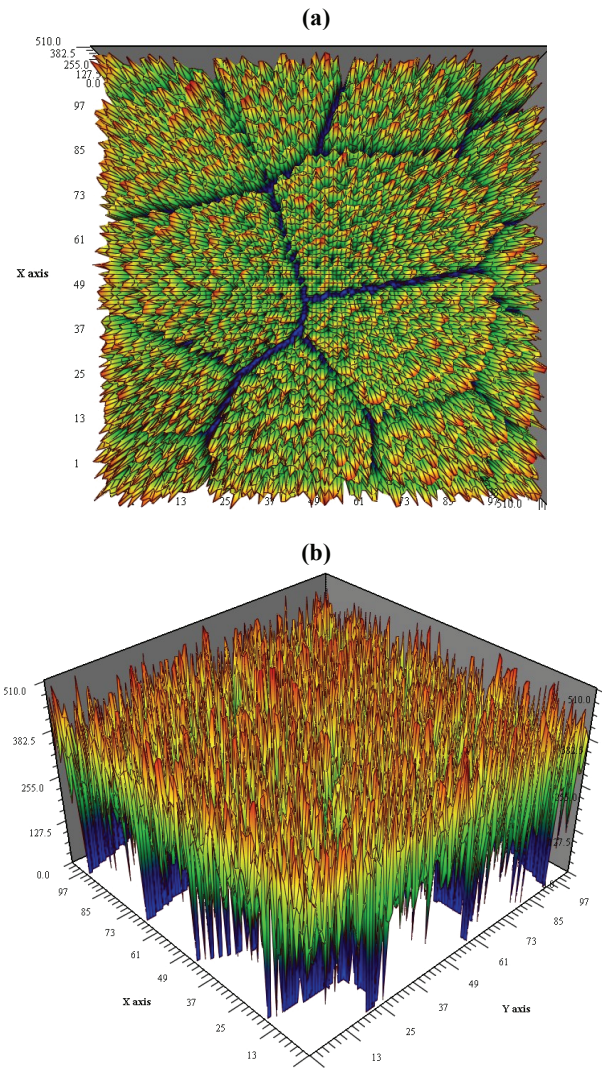

Fig. 10. *Initial dislocation distribution on the domain from (a) top view, (b) lateral view.*

The under-estimation comes from new grain boundary generation when a single cell as a new nucleus changes its state from the unrecrystallized to the recrystallized state. As described in the model assumptions, each grain is distinguished by a specific colour and a special digit. When a cell in a grain recrystallizes, it takes a new digit and a new colour to be distinguished from the surrounded unrecrystallized cells. Also, according to the model, the grain boundary is defined as one layer of cells between two different-coloured cells. Therefore, one layer of cells should be defined as a grain boundary. Since, it is not possible to define a "grain boundary" only for a single recrystallized cell, the cellular layer as the grain boundary should be considered in the next time step when the recrystallized cell grows. So, in each time step, there are some new recrystallized cells without any grain boundary around them and the volume fraction of the grain boundaries will be lower than their actual value and the volume fraction of cells will be higher than their actual value. So, the quota of each cell to accept new dislocations due to deformation will be lower and the whole dislocation density of the domain will decrease and under-estimation happens.

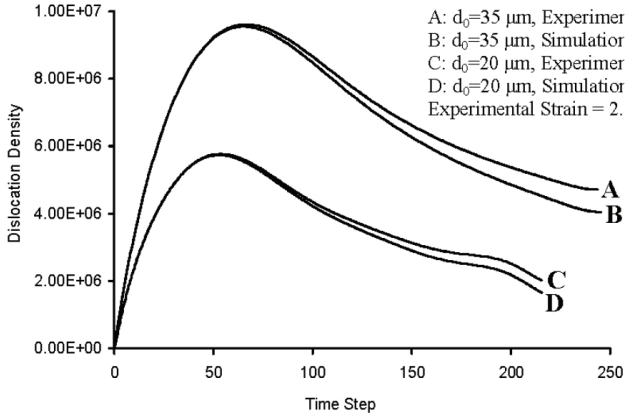

Fig. 11. *Experimental and simulation results with the initial grain size of 35 (A,B) and 20 micron (C,D).*

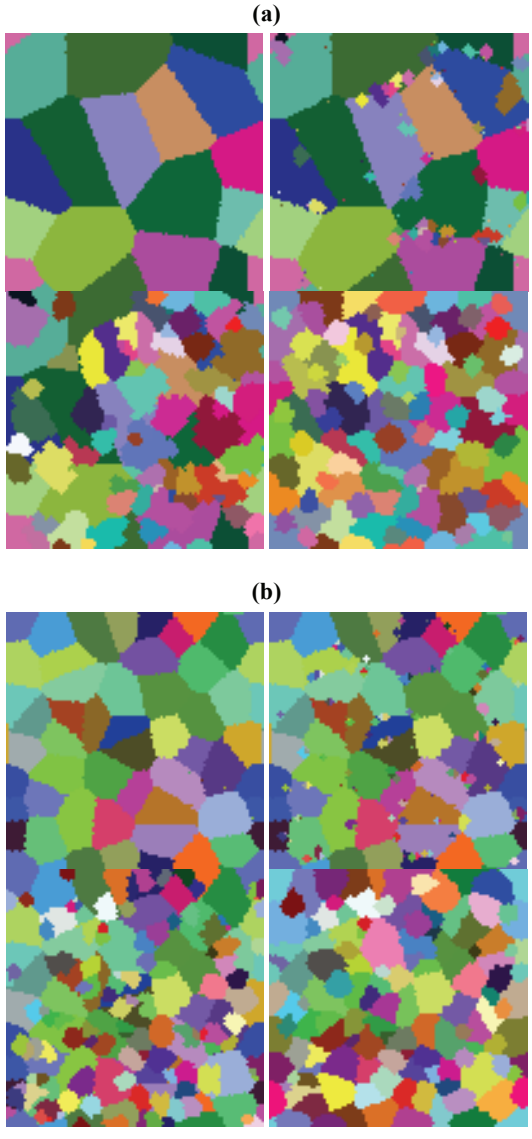

Fig. 12. *Microstructure evolution from the initial step of nucleation up to impingement with different initial grain size (a) d_0=35 micron, (b) d_0=20 micron.*

To further validate the model, the final grain size for the two different initial grain size was considered. The final grain size depends only on the temperature and strain rate. Therefore, two different initial grain size result in a similar final grain size. Figure 12 illustrates the microstructure evolution from an initial grain size of 35 μm and 20 μm respectively. The final grain size of the former condition is 10.7 μm while the final grain size of the latter condition is 10.3 μm. This means that the final grain size is independent of the initial grain size. This result conforms to the independence of final grain size from the initial grain size and therefore validates the current model.

5. CONCLUSION

Cellular automaton technique was employed to model DRX and its following microstructure evolution. According to the simulation results, the initial nuclei density is an important parameter during homogeneous recrystallization and it directly affects the final microstructure. Simulation results show good accord with ideal JMAK theory. The microstructure evolution seems to be accurate and a comparison between the simulated and experimental results indicates that the recrystallization behaviour is also properly described by this model. Also, it is shown that final microstructure depends on thermomechanical parameters including strain rate and temperature and the final grain size is independent of initial grain size. In addition, the CA model can be extended to different materials under various thermomechanical conditions by selecting the proper input data for each condition.

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MODELOWANIE REKRYSTALIZACJI DYNAMICZNEJ Z WYKORZYSTANIEM LOSOWEJ METODY AUTOMATÓW KOMÓRKOWYCH

Streszczenie

Symulacje komputerowe są doskonałym narzędziem umożliwiającym przewidywanie rozwoju mikrostruktury podczas rekrystalizacji dynamicznej. Automaty komórkowe są jedną z najbardziej efektywnych metod symulowania zjawisk fizycznych zachodzących podczas rekrystalizacji i rozrostu ziaren. W niniejszym artykule obydwa wymienione zjawiska zostały zamodelowane przy wykorzystaniu dwuwymiarowej siatki automatów komórkowych. Dane takie jak czas, wstępna wielkość ziaren oraz wstępna gęstość zarodkowania zostały wykorzystanie do walidacji modelu jako zmienne modelu JMAK (Johnson, Mehl, Avrami, i Kolmogorov). Zgodnie z przyjętymi założeniami, automaty komórkowe okazały się być dogodnym narzędziem symulacji zjawiska dynamicznej rekrystalizacji.

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