MODELLING MICROSTRUCTURE EVOLUTION DURING EQUAL CHANNEL ANGULAR PRESSING OF MAGNESIUM ALLOYS USING CELLULAR AUTOMATA FINITE ELEMENT METHOD

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Abstract

Equal channel angular pressing (ECAP) is one of the most popular methods of obtaining ultrafine grained (UFG) metals. However, only relatively short billets can be processed by ECAP due to force limitation. A solution to this problem could be recently developed incremental variant of the process, so called I-ECAP. Since I-ECAP can deal with continuous billets, it can be widely used in industrial practice. Recently, many researchers have put an effort to obtain UFG magnesium alloys which, due to their low density, are very promising materials for weight and energy saving applications. It was reported that microstructure refinement during ECAP is controlled by dynamic recrystallization and the final mean grain size is dependent mainly on processing temperature.

In this work, cellular automata finite element (CAFE) method was used to investigate microstructure evolution during four passes of ECAP and its incremental variant I-ECAP. The cellular automata space dynamics is determined by transition rules, whose parameters are strain, strain rate and temperature obtained from FE simulation. An internal state variable model describes total dislocation density evolution and transfers this information to the CA space. The developed CAFE model calculates the mean grain size and generates a digital microstructure prediction after processing, which could be useful to estimate mechanical properties of the produced UFG metal.

Fitting and verification of the model was done using the experimental results obtained from I-ECAP of an AZ31B magnesium alloy and the data derived from literature. The CAFE simulation results were verified for the temperature range 200-250 °C and strain rate 0.01-0.5 s^{-1}; good agreement with experimental data was achieved.

Key words: severe plastic deformation, equal channel angular pressing, ultrafine grained metals, magnesium alloys, cellular automata finite element method

1. INTRODUCTION

1.1. Cellular automata finite element (CAFE) method

Cellular automata (CA) technique is used in material science to provide digital representation of material microstructure and simulate its evolution during processing (Das, 2010; Madej et al., 2006;

Svyetlichnyy, 2012). Material is represented as a lattice of finite cells, called the cellular automata space. The interactions between cells describe dynamics of a simulated physical phenomenon. Mathematical description of interactions is introduced by transition functions (transition rules). The current state of each cell is determined by the state of its neighbours and its own state in the previous step. Cellular automata finite element (CAFE) approach is

the example of a multi scale modelling approach. This is the combination of micro scale modelling using cellular automata and finite element (FE) analysis, the most popular method of metal forming simulations. The advantages of using multi scale simulation approach are evident, especially when ultra fine grained materials are considered. By using the CAFE method not only the mean grain size but also microstructure homogeneity and grain size distribution can be calculated.

1.2. Equal channel angular pressing and its incremental variant

In order to improve mechanical properties of magnesium and other metals many thermo-mechanical processes have been proposed. Severe plastic deformation (SPD) processes, in which a very large strain is imposed to the material to refine its grain microstructure and improve its strength, are very promising. Equal channel angular pressing (ECAP) was developed by Segal (1995). In the ECAP process, a billet is pushed through a die with two channels, which have the same cross section (circular or rectangular) and intersect at an angle that usually varies from 90° to 135°. Plastic strain is introduced into metal by simple shear, which occurs at the channel intersection. Since the billet dimensions remain unchanged, the process can be repeated in order to accumulate a desired high strain.

Due to force limitation only relatively small amount of material can be processed at each stage. That is the reason why ECAP is not widely used in industrial practice. Recently, incremental ECAP (I-ECAP) has been developed by Rosochowski and Olejnik (2007). In I-ECAP, the stages of material feeding and plastic deformation are separated, which reduces the feeding force dramatically. The tool configuration consists of a punch working in a reciprocating manner and a die leading and feeding the material in consecutive steps. When the punch moves away from the die, the billet is fed by a small increment. Then, when feeding stops and the billet is in the fixed position, the punch approaches and plastically deforms it. The mode of deformation is simple shear, the same as in classical ECAP.

1.3. Microstructure evolution during ECAP of Mg alloys

Figueiredo and Langdon (2010) presented a model, which states that the mechanism of grain refinement during ECAP processing of AZ31 magnesium alloy is dynamic recrystallization (DRX). This hypothesis is based on the occurrence of a bimodal microstructure after ECAP processing. They also introduced a 'critical grain size' term in order to explain that homogenous grain size distribution is possible to achieve only if the initial mean grain size is small enough. Otherwise, the newly formed recrystallized grains are not able to fully consume the initial coarse grains. This observation was made earlier by other researchers (Janeček et al., 2007; Lapovok et al., 2008; Ding et al., 2009). Therefore, cellular automata transition rules usually used to describe DRX during hot forming of metals are applied in the presented model.

2. MODEL DESCRIPTION

2.1. Overview

In the present work, microstructure evolution during ECAP and its incremental variant is modelled using cellular automata finite element (CAFE) technique. The cellular automata (CA) space plays a role of digital material representation in meso scale; artificial grains are represented by CA cells. Microstructure evolution is described by transition functions, whose parameters are the macro scale integration point variables obtained from FE simulation: strain, strain rate and temperature (mapped from FE nodes). The internal state variable method (Pietrzyk, 2002), which treats dislocation density as a material variable, is used to describe changes that occur in the micro scale during plastic deformation. Dislocation density in each cell controls the nucleation process. Random pentagonal neighbourhood and absorbing boundary conditions are used to define CA space and its dynamics.

2.2. Dislocation density evolution

Evolution of dislocation density during hot metal forming is controlled by two competing processes: strain hardening and thermal softening caused by recovery or recrystallization. Increase in dislocation density is caused by storage of dislocations while decrease in dislocation density results from annihilation of dislocations. The change of dislocation densi-

ty due to strain increment is described by the equation (1) (Sellars and Zhu, 2000):

$$d\rho_i^{CA} = d\rho_i^{CA+} - d\rho_i^{CA-} =$$

$$A_1 \frac{M}{b} \dot{\varepsilon} \exp\left(\frac{Q_1}{RT}\right) d\varepsilon_i^{CA} - A_2 \rho_{i-1}^{CA} \exp\left(-\frac{Q_2}{RT}\right) d\varepsilon_i^{CA} \tag{1}$$

where: M – Taylor factor, b – Burgers vector, $d\varepsilon$– effective strain increment, Q_1 – effective activation energy, R – gas constant, T – temperature, $\dot{\varepsilon}$ – effective strain rate, ρ_{i-1}^{CA} – dislocation density at previous strain increment, Q_2 – apparent energy, A_1, A_2 – fitting parameters.

The presented approach is similar to the model developed by Mecking and Kocks (1981) where dislocation density evolution is also introduced as competition between dislocations storage and annihilation. Decrease in dislocation density is dependent on temperature as dislocation annihilation is characterized as thermally activated process (Madej et al., 2006).

Parameters of equations (1) were derived from literature (table 1). Fitting coefficients were determined using Hooke-Jeeves optimization method. Dislocation density dependence on strain at 200°C and strain rate equal to 0.01 s^{-1} based on these parameters, together with experimental results obtained for pure magnesium in similar conditions (Klimanek & Poetzsch, 2002; Mathis et al., 2004), are illustrated in figure 1.

2.3. Cellular automata space evolution

Microstructure evolution during processing is modelled using transition rules, which describe how each CA cell state changes depending on its own and its neighbour state after the previous time increment. The CA space dynamics can be described by the following rules:

– cell becomes the site of nucleation when its dislocation density exceeds a critical value; privileged areas for the dislocation density rise are grain boundaries and their vicinity (Galiyev et al., 2003);

– cell changes its state to recrystallized when one of its neighbours is recrystallized; grain grows until its virtual energy related to its grow potential is greater than zero; new grains cannot be consumed by other recrystallized grains.

A critical value of dislocation density in a CA cell must be reached to create a new grain nucleus in this cell. The nucleation process will be favoured where the level of stored energy is higher comparing to other areas. Following these arguments, the equation (2) is used to calculate critical dislocation density. This is a simplified form of the formula introduced by Roberts and Ahlblom (1978):

$$\rho_{crit} = \left(p_1 \dot{\varepsilon} T^{p_2} \gamma\right)^{1/3} \tag{2}$$

where: γ – grain boundary energy, p_1, p_2 – fitting parameters (table 2).

Table 1. *Parameters of dislocation density evolution equation (1).*

A$_1$	A$_2$	Q$_1$, kJ/mol (Barnett, 2003)	Q$_2$, kJ/mol (Das, 2010)	M, - (Chino, 2006)	b, nm (Chino, 2006)
3.85e3	30	147	21	2.38	0.32
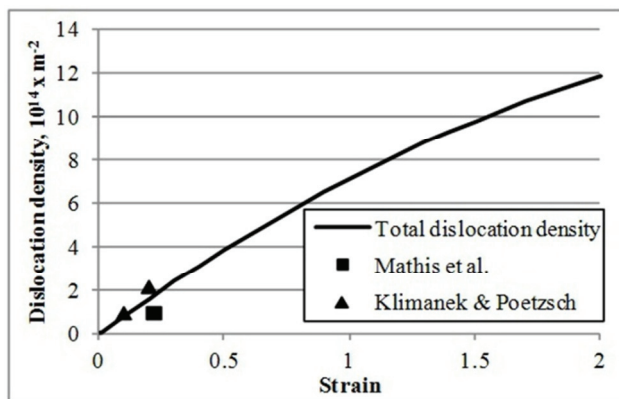
Fig. 1. *Dislocation density evolution at 200 °C and strain rate 0.01 s^{-1}.*

Grain boundary energy is dependent on the misorientation angle between neighbouring grains and is evaluated from the equation derived by Read and Shockley (1950) for low angle grain boundaries; for high angle grain boundaries it is kept constant. Misorientation between neighbouring grains is calculated using a method presented by Zhu et al. (2000).

Orientation of each grain is described by three Euler angles: φ_1, Φ, φ_2 (Bunge notation). Wang and Huang (2003) showed the relation between crystallographic orientation and texture component in hcp metals. Since the slip on basal plane is the most favourable deformation mechanism for magnesium, dislocation accumulation is more probable for grains with orientation closer to basal than prismatic or

pyramidal one. Processing at elevated temperatures is being simulated, therefore twinning is not taken into account. Moreover, twinning was not revealed in microscopic observations.

At each time step, the total dislocation density increment is divided by a number of randomly chosen cells N, which extrinsic dislocation density will be increased. The parameter is dependent on temperature and strain rate obtained from FE simulation. Since grain boundaries are prevailed areas for nucleation, more new nuclei are expected to occur when there are more grains in the CA space. Evolution of N is given by equation (3):

$$N = p_3 \dot{\varepsilon}^{p_4} n_d^{p_5} \exp(p_6 T) \qquad (3)$$

where: N – number of cells with increased extrinsic dislocation density, n_d – number of grains in CA space, p_3, p_4, p_5, p_6 – fitting parameters.

Grain growth rate is associated with virtual energy assigned to each new nucleus. Since mean DRXed grain size is dependent mostly on temperature, grain growth energy is the function of temperature and misorientation angle. As the new grain grows its energy is being lowered. The process is stopped when the grain growth energy is equal to zero. In this condition, the grain has no potential for further expansion. The grain growth energy is introduced using an empirical equation (4):

$$E_{gg}^{grain} = p_7 \exp(p_8 T)(10/\theta + 0.7) \qquad (4)$$

where: T – temperature, θ – misorientation angle, p_7, p_8 – fitting parameters.

Table 2. *Parameters of CA space evolution equations (2-4).*

p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8
4.0756e70	-31.4176	0.6677e18	0.004261	1.06699	-0.092	1.1463	0.094

3. EXPERIMENTAL PROCEDURE

Commercially extruded AZ31B magnesium rods with 17 mm diameter were machined using the EDM cutting technique in order to obtain bars with square cross-section 10 x 10 mm^2 and length equal to 100 mm. A double-billet variant of I-ECAP was realised using a 1 MN hydraulic servo press (Rosochowski et al., 2008). The billets were fed using a screw jack whose action was synchronised with the reciprocating movement of the punch. The punch movement followed an externally generated sine waveform with frequency 0.5 Hz and amplitude equal to 1.8 mm. A motor driven screw jack was controlled using National Instruments hardware and software (LabVIEW). The feeding stroke was equal to 0.2 mm.

A die with 90° angle between channels was used to conduct four passes of I-ECAP, which resulted in the total strain of 4.6. Route B$_C$ was used, which meant that after each pass the billet was rotated by 90°. AZ31B billets and dies were heated up to 250°C using electric heaters. Temperature during processing was kept constant within ±2 °C, based on the readings obtained from a thermocouple located near deformation zone.

4. RESULTS

FE simulations were run using Abaqus/Explicit commercial software. CA microstructure evolution calculations and visualisation were performed using a self-developed software. CA space dimensions were 400 x 400 cells, it corresponded to 100 x 100 μm^2 area of real material. The same conditions as during I-ECAP experiment were used in simulation. In order to investigate temperature and strain rate effect on the final mean grain size and microstructure homogeneity, additional experimental results obtained for different process parameters were derived from literature (table 3). Simulations were performed for temperatures: 200, 225 and 250°C and strain rate within range 0.01-0.5 s^{-1}.

The initial microstructure of I-ECAP processed material was heterogeneous; coarse grains were surrounded by smaller ones (figure 2a), what could be attributed to DRX during hot extrusion of supplied rods. The corresponding digital representation of as-received material was obtained by uniform grain growth and simulation of DRX (figure 2b). The mean grain size obtained after I-ECAP processing was equal to 6.15 μm (figure 2c) what is similar to the results obtained by Suwas et al. (2007). Strain rate values during both processes were significantly different, which could indicate that processing temperature has a dominant effect on the final grain size. The simulated microstructure was similar to the real one and the predicted grain size was 6.3 μm (figure 2d).

**Table 3.** *Simulations parameters.*

	Initial temperature, °C	Strain rate, s^{-1}	Channel angle, °
I-ECAP (this work)	250	0.5	90
Ding et al. (2009)	225	0.3	120
Ding et al. (2009)	200	0.3	120
Jin et al. (2006)	225	0.01	90
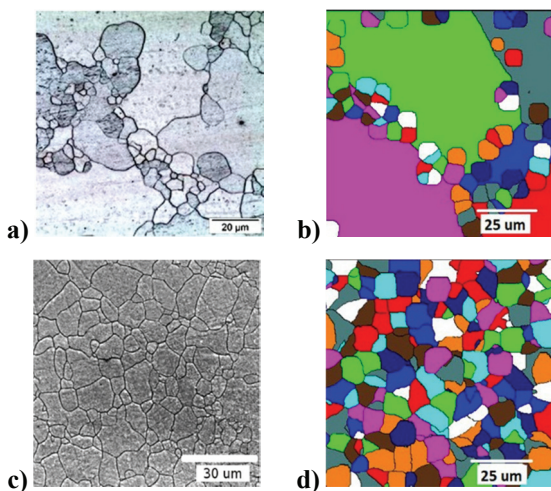
Fig. 2. *Microstructure images of as-received material (a) and after 4th pass of I-ECAP at 250 °C (c); corresponding simulation results in (b) and (d), respectively.*

Ding et al. (2009) conducted ECAP of AZ31 magnesium alloy at 200°C and 225°C using a die with 120° channel angle. The initial microstructure and its digital material representation are shown in figure 3. The initial mean grain size was 7.2 μm, the same as the average grain size of CA representation. The microstructure obtained after 4 passes at 200°C and the corresponding results of modelling microstructure evolution are shown in figure 3 as well. After 4 passes at 200°C the grain size was reduced to 1.8 μm while the model predicted 1.7 μm. When processing at 225°C, the microstructure was less homogenous than at 200°C. The mean grain size calculated using developed model was equal to 2.2 μm, while experimental result was 2.4 μm.

The initial mean grain size of the material processed by Jin et al. (2006) was equal to 15.6 μm; coarse grains and few smaller grains were observed (figure 4a). A digital material representation was generated using non-uniform grain growth: 80% of grains grew slower than others and the mean grain size was 15.8 μm. After first pass at 225°C, coarse grains were surrounded by colonies of very small

grains (figure 4c). The interior of coarse grains was not consumed during DRX process. The mean grain size after first pass was measured to be 4.1 μm while the model predicted 4.25 μm.
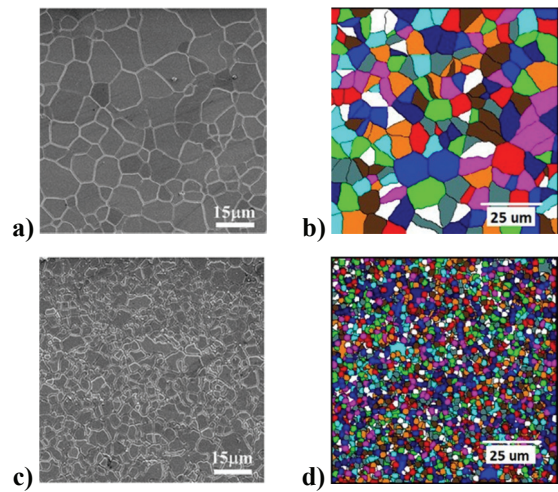
Fig. 3. *Microstructure images of as-received material (a) and after 4th pass of ECAP at 200 °C (c) obtained by Ding et al. (2009); corresponding simulation results in (b) and (d), respectively.*
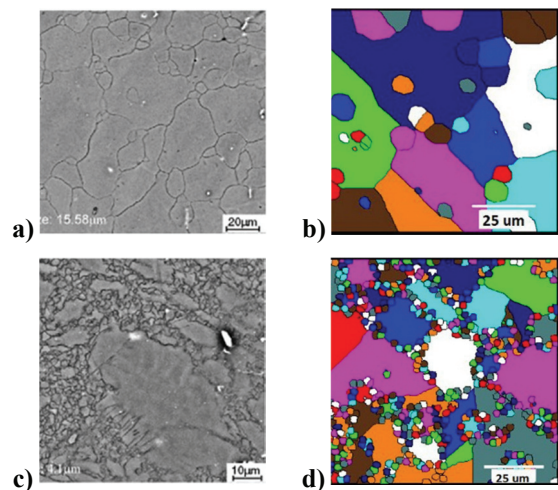
Fig. 4. *Microstructure images of as-received material (a) and after 1st pass of ECAP at 225 °C (c) obtained by Jin et al. (2006); corresponding simulation results in (b) and (d), respectively.*

Results obtained from the developed CAFE model are in good agreement with experimental data (figure 5). The mean grain size after first pass depends strongly on the initial microstructure. A significant grain refinement is observed after first pass but it is not sufficient to refine the coarse grain dominated microstructure. Only grains smaller than ~15 μm can be fully recrystallized during first pass of ECAP at 200°C. As a result, heterogeneous grain size distribution is obtained. Further deformation is needed to refine and homogenize a microstructure. Grain refinement is limited by a temperature, it is

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shown that the mean grain size as small as 2 μm can be obtained at 200°C. Although smaller grain size cannot be obtained at given temperature, further processing leads to microstructure homogenization.
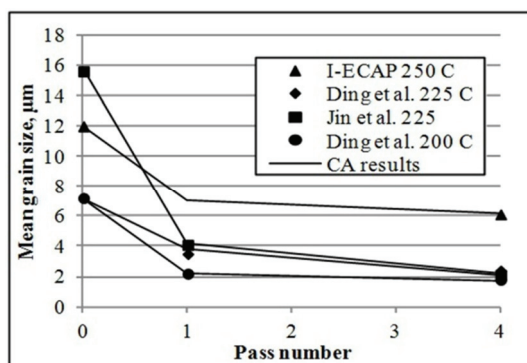

Fig. 5. *Mean grain size obtained from experiments and CAFE simulations.*

5. CONCLUSIONS

A multi scale CAFE approach was developed in order to model microstructure evolution during equal channel angular pressing. Computations were performed for various temperatures and strain rates that are typical for processing of magnesium alloys. Numerical results were verified using experimental data from conventional and incremental ECAP. Former were derived from literature, latter was obtained from I-ECAP experiment. The model correctly predicted both the mean grain size after subsequent passes of ECAP/I-ECAP and microstructure homogeneity. In particular, a heterogeneous grain size distribution after first pass of ECAP for initially coarse grained microstructure was predicted as well as its further homogenization. Future work will be focused on modelling grain reorientation due to deformation by simple shear.

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MODELOWANIE ROZWOJU MIKROSTRUKTURY PODCZAS RÓWNOKANAŁOWEGO WYCISKANIA KĄTOWEGO STOPÓW MAGNEZU PRZY UŻYCIU METODY CAFE

Streszczenie

Równokanałowe wyciskanie kątowe (*equal channel angular pressing – ECAP*) jest jedną z najpopularniejszych metod otrzymywania ultra drobnoziarnistych metali. Jednak z powodu dużych sił potrzebnych do przeprowadzenia procesu, tylko relatywnie krótkie wstępniaki mogą być wyciskane. Rozwiązaniem problemu może być opracowany inkrementalny wariant tego procesu, tzw. I-ECAP. Ze względu na to, że przy użyciu I-ECAPu mogą być przetwarzane nieskończenie długie elementy, może on znaleźć szerokie zastosowanie w praktyce przemysłowej. Mechanizm rozdrobnienia ziarna podczas przeróbki plastycznej stopów magnezu różni się znacząco od metali takich jak aluminium lub miedź i ich stopy. Ostatnie wyniki wskazują, że mechanizm rozdrobnienia ziarna podczas ECAPu jest sterowany przez proces rekrystalizacji dynamicznej, a ostateczna średnia wielkość ziarna jest zależna głównie od temperatury procesu.

W niniejszej pracy sprzężona metoda automatów komórkowych i elementów skończonych (*cellular automata finite element – CAFE*) została wykorzystana do opisu rozwoju mikrostruktury podczas czterech przejść ECAPu i jego inkrementalnego wariantu, I-ECAPu. Dynamika zmian w przestrzeni automatów komórkowych jest determinowana przez reguły przejścia, których parametrami są odkształcenie, prędkość odkształcenia oraz temperatura – uzyskane z symulacji metodą elementów skończonych. Model zmiennej wewnętrznej opisuje wzrost całkowitej gęstości dyslokacji i przekazuje tę informację do przestrzeni automatów komórkowych. Opracowany model CAFE oblicza średnią wielkość ziarna oraz generuje cyfrowy obraz mikrostruktury, co może być przydatne w wyznaczaniu własności mechanicznych otrzymanego materiału.

Dopasowanie oraz weryfikacja modelu zostały wykonane przy wykorzystaniu wyników uzyskanych z przeprowadzonego procesu inkrementalnego ECAPu stopu magnezu AZ31B oraz danych literaturowych. Wyniki symulacji metodą CAFE zostały zweryfikowane dla zakresu temperatur 200-250°C oraz prędkości odkształcenia 0.01-0.5 s^{-1}; uzyskano bardzo dobrą zgodność z wynikami eksperymentalnymi.

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