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MODELING WITH FCA-BASED MODEL OF MICROSTRUCTURE EVOLUTION IN ULTRA-THIN WIRES OF MGCA08 ALLOY DURING HOT DRAWING

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Summary. Magnesium alloys are widely applied in medicine due to their high biocompatibility and solubility in human body. For example, they could be applied for surgical threads used for integration of tissue [1,2]. This application requires wires diameter of 0.1 mm and smaller. A new manufacturing process of thin wires, including drawing in heated dies, was developed by Authors [3,4] for biocompatible Mg alloys. An occurrence of recrystallization is the main condition of such a process, which does not use intermediate annealing between the deformations. Because the trial and error method is very expensive and ineffective, a numerical modeling was applied for process design and its optimization. A model of recrystallization of MgCa0.8 alloy in macro scale was developed previously [5]. This model allows for prediction and optimization of drawing process parameters. However, basing on the results of the study [5], we conclude that some microstructural phenomena should be additionally considered in the case of ultra-thin wire drawing in the heated tools. An analysis of the effect of the wire diameter on recrystallization kinetics was an object of interest, especially when wire diameter is comparable with grain size. Study of influence of such a geometrical parameter was fulfilled with use of FCA-based model. The modelling shows that an approaching of the wire diameter to the grain size elongates the recrystallization process with other conditions the same. For example, a decrease of the diameter from 200 to 20 μm extends the recrystallization time by 30%. From the practical point of view, the results detached such a geometrical parameter can be implemented into simpler models of recrystallization, e.g. JMAK-based models.

1 INTRODUCTION

Magnesium alloys are applied in medicine for sake of high compatibility and solubility in human organism [1,2]. Production of surgical threads used for integration of tissue may be one of the applications of those alloys types [2,3]. This application requires wires with diameter

about 0.1 mm. Magnesium alloys are very difficult for deformation, which is connected with their hexagonal close packet structure. That is why a new manufacturing technology of wire drawing process in heated dies assisted with numerical model was developed [4,5]. This technique is designed especially for thin magnesium wires with diameter less than 1.0 mm. According to this technology the drawing process performed in conditions where the recrystallization occurs in every draft. In this case it is possible to carry out multi-pass process without annealing.

Model of recrystallization of MgCa0.8 magnesium alloy in macro scale was developed and presented in [6]. This model allows for quick prediction and optimization of drawing. However, the results presented in [5,7] suggest that the impact of the thermo-mechanical processes, occurring in the micro scale is essential, especially for the thin wire. For this reason, in the present study, the recrystallization process is considered in the micro scale using the cellular automata (CA) model.

CA-based models is a very useful and universal tool for the simulation of microstructure evolution. Crystallization (solidification) [8–11], dynamic and static recrystallization [12-17], phase transformation [12, 18–21], grain refinement [22-26] and other microstructural phenomena are successfully modelled with use of CA. One of the possible modifications of the CA, known as Frontal Cellular Automata (FCA) [14], which allows for an algorithmical reduction of the calculation time, is used in this paper.

A hierarchical system based on FCA for modelling of microstructural phenomena and technological processes was developed [25]. A general block-scheme of the system presented in figure 1.

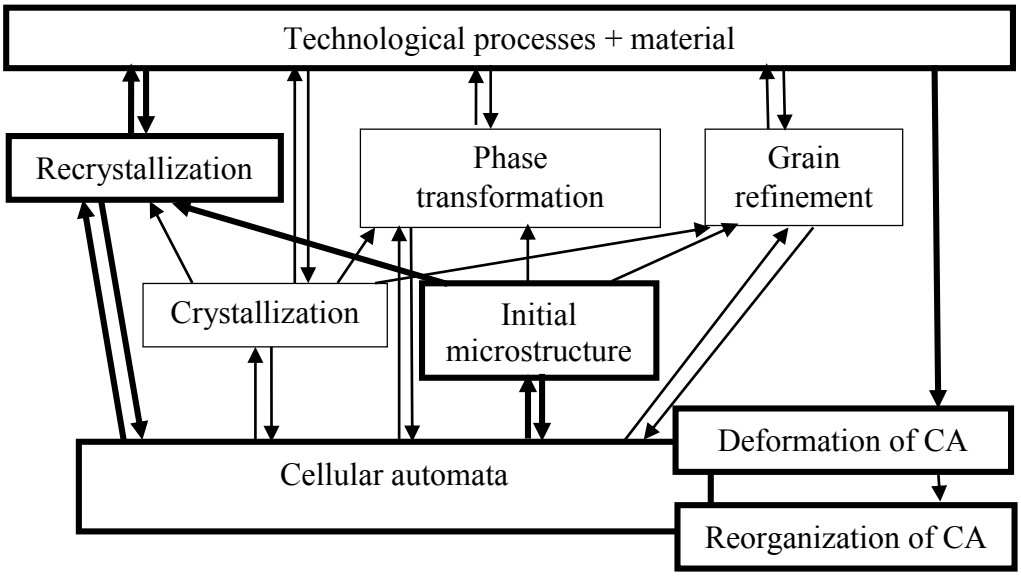

Figure 1: FCA-based model for simulation of microstructure evolution in technological processes

The basis of this system is FCA, while the top is a set of processes. Models of microstructural phenomena are between them and connect them. The database of materials completes the system. Bold lines mark the modules and proper connections are used in the present study.

Frontal cellular automata and its computational advantages are described in detail elsewhere [14, 19, 21, 25]. Additionally, detailed information about consideration of the deformation in FCA and space reorganization can be found in [19, 27, 28]. Results of modelling and simulation with this FCA-based system are presented elsewhere: solidification in continuous casting [11], hot flat and shape rolling [21, 27,29, 30], the roll-bonding process and MAXStrain technology [25, 26], powder bed generation, etc.

The goals of present work are the development and validation of FCA-base model of microstructure evolution of MgCa0.8 magnesium alloy.

2 GEOMETRICAL MODELING WITH FCA

Processes modeled later have feedback on parameters of the initial microstructure. It means that not only material parameters (grain sizes, crystal lattice, texture, etc.) should be taken into account but also the condition of further space reorganization must be considered. The initial microstructure for further modeling was created in three stages [28]: choice of the shape of the grains, creation of the structure for a given grain size distribution and adjustment of crystallographic parameters.

The microstructure of very thin wire is shown in figure 2. The wire sizes are comparable with grain size. Here, the periodic boundary conditions are applied for face-end surfaces and the open conditions for the other surface. The material of the wire is MgCa0.8 magnesium alloy with hexagonal crystal lattice, and the shape of the growing grains was a hexagonal prism with axis orientated almost radially to the axis of the wire. The dimensions of the initial representative volume are $x \times y \times z = 200 \times 100 \times 100$ μm, with cellular space $n_x \times n_y \times n_z = 400 \times 200 \times 200$ cells.

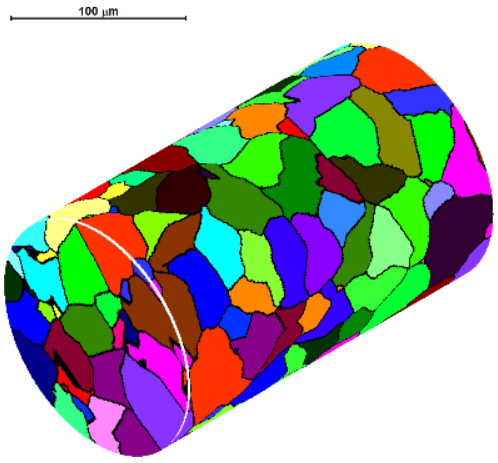

Figure 2: Initial microstructures before passes

Some variants of crystallographic orientation distribution can be applied in FCA [28]: uniform distribution of all angles, uniform distribution on the sphere and normal (Gaussian) distribution for the Euler angles. The last variants was used in present simulations. This distribution is shown in inverse pole figures (figure 3) for microstructure presented in figure2.

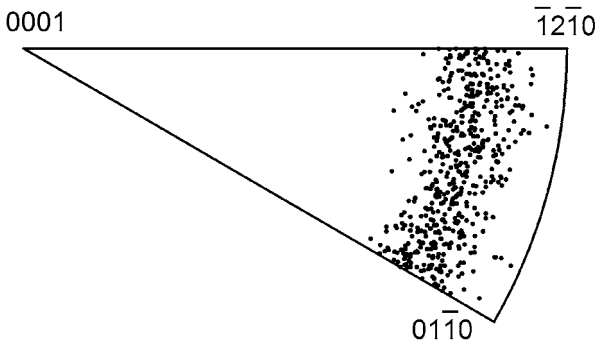

Figure 3: Inverse pole figure for textured microstructure.

The microstructure was prepared for thin drawing wire for further modelling of fracture [7], drawing with recrystallization [5] and use with FEM-BEM (boundary element method) code [3]. The material is of hexagonal crystal lattice. Then, distributions of three Euler rotation angles were chosen, as described below. During the deformation, the lattice rotates in such way that the angle between the hexagonal axis and the direction of maximal compression approaches an angle of 10 degrees. Because this hexagonal axis is initially set with the drawing direction, the second Euler rotation angle should be about 80° (a Gaussian distribution with a mean value 80° and a standard deviation of 3° is chosen for this rotation angle). Because compression during the drawing is directed to the axis of the wire, the hexagonal axis of the lattice should go through the axis of the wire. This condition determines the first Euler rotation angle. Then, the first Euler rotation angle should agree with the location of nuclei. Therefore, there is the uniform distribution of the third Euler rotation angle (0 ÷ 360°); Gaussian distribution with a mean value of 80° and standard deviation of 3° for the second Euler angle; and the first rotation angle depends on the nucleon location in such a way, that after the second rotation, the first rotation axis goes through the axis of the wire.

After the microstructure was created (figure 2), the wire was elongated (figure 4 and 5). The initial diameter was 0.1 mm, and after drawing, 0.08 mm. Two variants microstructure after the two passes are presented in figures 4 and 5 for comparison. The first microstructures (figure 4) demonstrate only grain deformation without consideration of microstructure evolution. The second microstructures (figure 5) were obtained during the modeling of the drawing process with simulation of cDRX (continuous dynamic recrystallization). Effect of cDRX can be observed for several grains, which were split on parts, while the most others saved their shapes and sizes. Some grain refinement is the result of cDRX.

However cDRX is the process considered for the cold deformation mainly. It can be observed during the hot deformation, as well. But discontinuous dynamic (dDRX), metadynamic (MDRX) and static recrystallization (SRX) are predominated. Then, FCA-based model consider all the types of recrystallization together. During the deformation cDRX and dDRX act concurrently. Dislocation cells, subgrains and new grains are developed along with new nuclei appearance. Then, after the deformation, MDRX and SRX form microstructure on the background of static recovery.

Small wire diameter allows us to assume the low differences in temperature, almost the same conditions of nucleation and grain grow in all wire cross-section. Then, all process variables can be applied globally for whole material. It mean, that the final microstructure (geometrically)

can be considered independently from the recrystallization kinetics. Local effect of temperature heterogeneity on the nucleation and grain growth and consequently the microstructure can be neglected.

Results of microstructure simulation after complete recrystallization are presented in figure 6. Effect of elongated grains is disappeared.

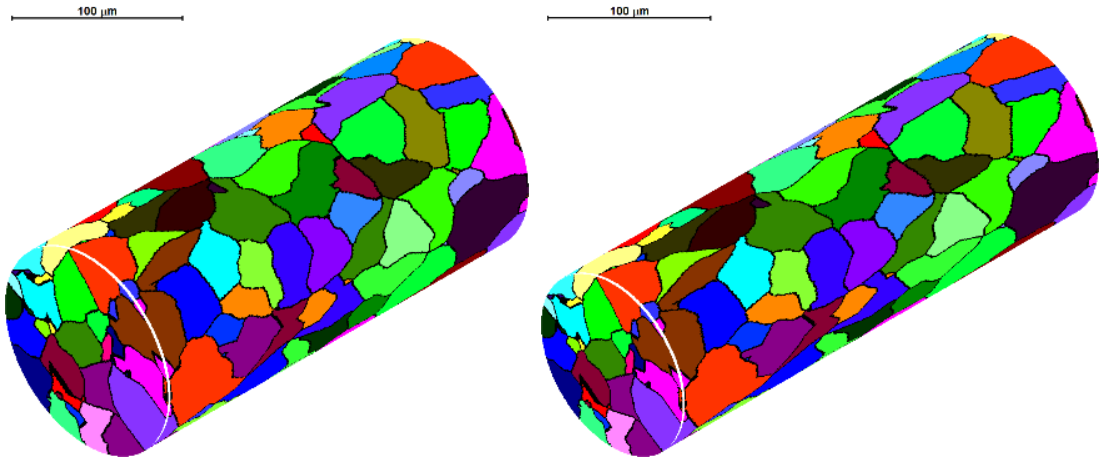

Figure 4: Microstructures before (a) and after the last pass without cDRX

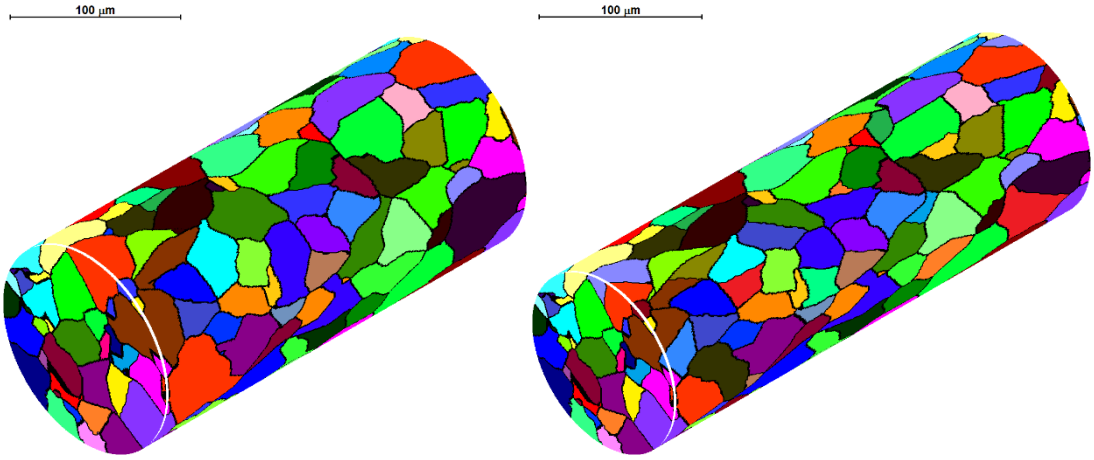

Figure 5: Microstructures before (a) and after the last pass with cDRX

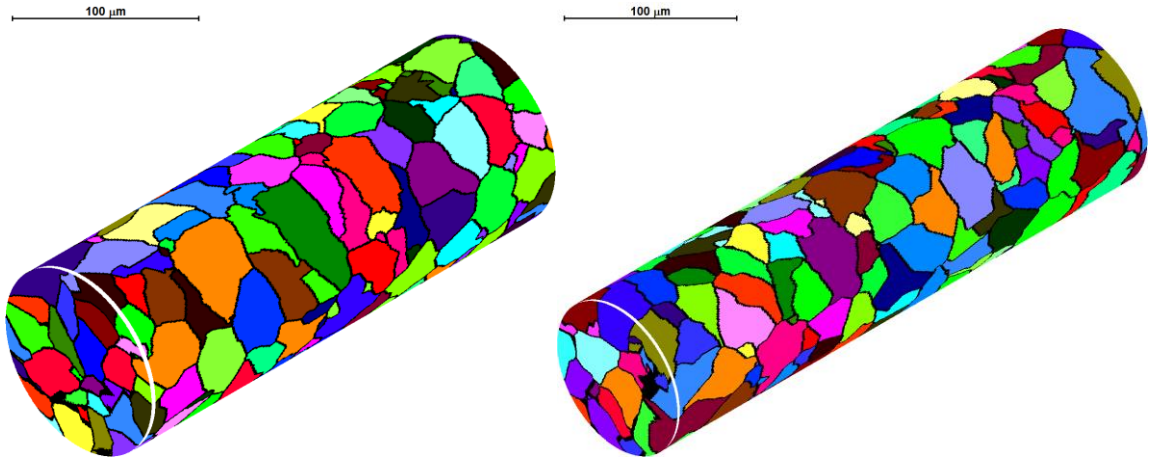

Figure 6: Microstructures before (a) and after the last pass with complete recrystallization

3 KINETICS OF RECRYSTALLIZATION

Results of an analysis of the effect of the wire diameter on recrystallization kinetics are presented in this section. When dimensions of specimen are significantly higher than grain size, this effect can be neglected. But, when wire diameter is comparable with grain size, kinetics cannot be considered without open boundary condition. Boundary effect is not only difference of deformation condition and temperature. Wire surface is an area, where grain growth is not limited with other grains growing in opposite direction. Thus, grains near the surface can grow more coarse than the grains far from the surface. Time of growth of surface grain is elongate because of their bigger size as well. Hence, recrystallization is slower.

It can be recalled, that recrystallization kinetics depends on several factors – temperature, dislocation density, etc. A geometrical factor is one of the others. For proper consideration of an effect of the geometrical factor on recrystallization kinetics, it should be studied separately from the others. Perhaps, it cannot be studied experimentally, but numerically with FCA-based model.

The geometrical parameter can be defined as ration of wire diameter to average grain size. Specific numbers are not important in the study of influence of such a geometrical parameter. Wire diameter, average grain size, grain growth rate, shape of growing grain and other parameters can be arbitrary. However, in the study these numbers were taken about real numbers of considered technology. The average grain size is 25 µm, diameter is 20 to 200 µm (minimal diameter of the wire in real process was 100 µm), grain growth rate is correspondent to 300°C. Cellular automata contain $n_x \times n_y \times n_z = 600 \times 300 \times 300$ cells. Representative volume is determined by diameter D and length L of wire: $L = 2\ D$. Volume and average grain size allows to calculate number of grain. Then nuclei are distributed randomly and new grains begin to grow.

The recrystallization kinetics is presented in figure 7. The modelling shows that an approaching of the wire diameter to the grain size elongates the recrystallization process with other conditions the same. For example, a decrease of the diameter from 200 to 20 µm extends the recrystallization time by 30%. However, effect of geometrical factor on the recrystallization

kinetics is small in the real range (wire diameter over 100 μm).

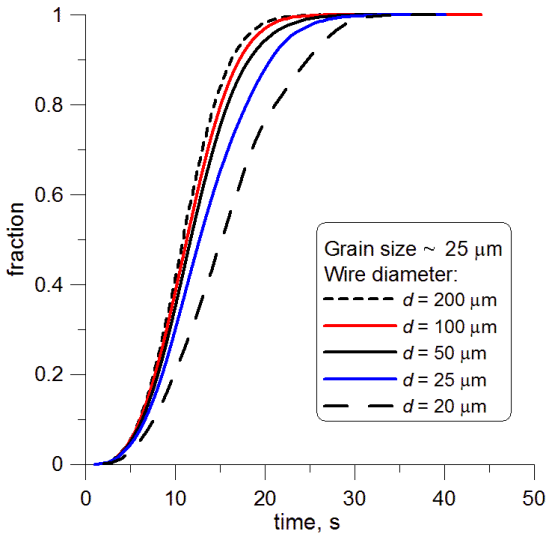

Figure 7: The recrystallization kinetics for temperature of drawing 300°C

4 CONCLUSIONS

- FCA-base model was developed for simulation of recrystallization during the drawing of thin wire in heated dies.
- Geometrical modelling of recrystallization was carried out. Model take into account real deformation, continuous and discontinuous dynamic, meta-dynamic and static recrystallization at varying temperature.
- The effect of the wire diameter on recrystallization kinetics was analysed. It is very important, when wire diameter is comparable with grain size.

Results of the study will be used for optimization of the developing drawing process of thin wire of MgCa0.8 alloy.

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