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Three-dimensional frontal cellular automata modeling of the grain refinement during severe plastic deformation of microalloyed steel

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ABSTRACT

In the current work, a computer model based on three-dimensional Frontal Cellular Automata (FCA) for the simulation of grain refinement during multiaxial compression was developed. The strong grain refinement obtained in microalloyed steel through subdivision of the initial coarse-grained structure into dislocation substructure and subsequently into stabile UFG structure was simulated and analyzed by FCA. Proposed in the present study model is a step forward toward understanding deformation mechanisms occurring during metal forming processes with high energy accumulation. Conclusions regarding possibilities of proposed numerical tool were drawn basing upon qualitative and quantitative comparisons of the modeling and SEM/EBSD results. Results obtained with FCA-based model were compared with SEM/EBSD results of real process and demonstrated a good agreement. A description of the model, results and conclusions are presented in the paper as well.

1. Introduction

Mechanical and physical properties of metals are determined by their chemical composition and microstructure that, in turn, is a result of a range of strengthening mechanisms, as an effect of deformation/heat treatment. However, a grain refinement still remains one of the best ways to achieve the superior properties such as high strength, good toughness, as well as good high and low cycle fatigue performance. Therefore, over the last few decades, there has been a considerable interest paid to ultrafine-grained (UFG) and nanostructured metallic materials aimed at numerous applications and various branches of the industry. Nowadays, these materials can be fabricated both under laboratory and industrial conditions. The processing techniques can be divided into two major approaches: bottom-up and top-down. The first ones include electro-deposition or various compaction methods. The top-down techniques are more important from the point of view of industrial applications. In this case, UFG/nanostructured materials are produced from a coarse-grained initial state using Advanced Thermomechanical Processing (ATP) [1–3] or Severe Plastic Deformation (SPD) [4–7]. The ATP methodologies involve existing industrial processes (mostly rolling) using microstructural phenomena, e.g. in the case of steel, dynamic austenite recrystallization with subsequent phase transformation, dynamic strain-induced ferrite transformation, intercritical rolling, warm rolling, reverse transformation, and cold rolling with subsequent annealing of martensitic starting microstructure. The SPD methods, in turn, as a main factor, use a large accumulative plastic strain at ambient temperature or warm deformation conditions. This group of techniques includes, first of all: Equal Channel Angular Pressing and Extrusion (ECAP, ECAE), Accumulative Roll Bonding (ARB), High Pressure Torsion (HPT) and multiaxisial compression. In these processing methods, applied severe plastic deformation causes a subdivision of the initial coarse-grained microstructure into dislocation cells and subgrains. At the beginning of the SPD processing, the microstructures are characterized by a high volume fraction of Low Angle Grain Boundaries (LABs). Then, due to the continuous dynamic recrystallization (recrystallization *in situ*) these LABs transform into more stable High Angle Grain Boundaries (HABs) [8–13].

Most of the SPD methods impose complex deformation modes that make the prediction of the microstructure evolution extremely difficult, mainly due to a high microstructural inhomogeneity that is introduced during multiple strain reversals. Thus, a concurrent effect of different elements of dislocations structure governs the microstructure evolution. Additionally, interactions between dislocations, LABs and HABs constantly change the overall hardening effect. Therefore, it is very difficult to determine a contribution of particular elements of the microstructure to the final material properties. So far, a computer modeling of microstructure evolution during SPD processes has been really difficult due to a lack of proper numerical tools that allow representing these high energy dislocation structures numerically. Recently, Digital Material Representation (DMR) has been proposed and widely used in computer

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simulations of deformation processes, microstructure evolution and finally, prediction of the material properties [14].

The possibility of prediction of the microstructure evolution in the micro-, meso- and macro-scale is one of the most important problems in materials science. Cellular automata (CA) models [15] occupy the first place among the methods used in the computer modeling of microstructure evolution. CA are used for modeling of crystallization (solidification) [16–20], dynamic and static recrystallization [21–25], phase transformation [23,26–29], grain refinement [30–33], etc.

CA-based models, which can be found in literature, usually are two-dimensional (2D). 2D CA models are simpler and faster, because they consist of fewer elements and connections, use more clear algorithms, and are much simpler for designing, implementation, as well as, more useful for visualization. The real microstructure, however, is not 2D in nature. Nevertheless, for simplification, there have been many numerical parameters introduced and effectively used in the microstructural analysis, e.g. the average grain size. Another parameter frequently used in the microstructural analysis describes the grain shape, which can be often represented by a residual strain or by the ratio of the grains volume to their surface area. A crystallographic orientation of grains and subgrains is the next feature that can be used to describe the presence and degree of the texture. One more subject of interest is the distribution of boundaries disorientation angle and its changes during the deformation. As mentioned above, the microstructure evolution is pointedly three-dimensional and results obtained by the 2D CA can never correspond to the real 3D processes. At least five main problems, partly unresolved, appear during the 2D CA modeling i.e.: kinetics of transformation, location of nuclei, grain growth rate, deformation of grains and crystallographic orientation. Some of them were investigated elsewhere in detail [20,29,33]. 3D CA are free of these problems, however, they are more complex and require much more time and memory for simulations. One of the possible modifications of the CA, known as Frontal Cellular Automata (FCA) [24], which allows for an algorithmical reduction of the calculation time, is used in this paper.

Recently, Authors used FCA to predict grain refinement that was presented in publications [30–33]. Conception of FCA application was described in details in the first of these publications [30], then three models were developed, simulated and discussed [31]. The results presented in Fig. 6 in [31] do not take into account real process of deformation and the model chooses slip plains and slip directions arbitrary. Later, the effects of deformation were distributed on slip planes and slip directions according to the crystal plasticity theory, which was implemented into the model [32]. In publication [33] are summarized the results, that were previously obtained; and two processes – ARB process (accumulative roll-bonding) and multiaxial compression (using MaxStrain deformation) are presented. ARB process is similar to flat rolling from the point of view of the state of deformation. It can be considered as a case of plane strain. This process was simulated for aluminum [33].

MAXStrain is one of the Mobile Conversion Units of Gleeble Systems, thermal–mechanical physical simulation and testing systems designed and manufactured by Dynamic Systems, Inc. The system restrains specimens lengthwise while allowing unlimited deformation in the other two dimensions, that is, a deformation process in the state of plane strain. A cycle is of two deformations, in which two axes are replaced. Elongation is replaced by compression, and vice versa. Then, the specimen after each cycle is back to its initial size, but the material accumulates strain. Some results of the computer simulation of two cycles MaxStrain deformation are presented in [33,39]. The first publication [33] considers an appearance of new boundaries only, without evolution of boundary disorientation. The second publication [39] considers the module of the initial microstructure taking into account the grain refinement. The initial microstructure was obtained in three stages: modeling the initial coarse microstructure – (a), the grain refinement according to required grain (subgrain) size distribution – (b) and fitting the disorientation boundary angle to the required distribution – (c).

In the present work, the appearance of new boundaries and rotation of dislocation cells (subgrains and grains) are simulated simultaneously. Moreover, rotation rate is set in such a way that parameters of the simulated microstructure were close to data from EBSD study. That was the identification simulation. It allowed one to conclude that the rotation rate decreases from cycle to cycle, especially that it drops quickly in the first cycle.

The objectives of the present work are experimental studies of the effect of the multiaxial compression on the grain refinement in microalloyed steel using MaxStain system [34] and an analysis of the evolution of the initial coarse microstructure into the ultrafine-grained structure with the use of three-dimensional FCA.

2. Experimental study of microstructure evolution during multiaxial compression

In the present study, the MaxStrain® system [35] was used to produce an ultrafine-grained microstructure during multiaxial compression test. In this test, each deformation cycle consists of two compressive deformations, in which the longitudinal axis of the specimen is constrained so the deformation energy is accumulated only in the deformation zone between two anvils. After the first deformation pass, the specimen is rotated by 90° around its longitudinal axis; and the second deformation is applied. This cycle can be repeated many times, so severe accumulation of the deformation energy can be reached without a loss of the specimen's integrity.

In the current investigations, multiaxial compression was carried out on a microalloyed steel with the following basic chemical composition [wt%]: 0.07C–1.36Mn–0.27Si–0.067Nb–0.073Ti–0.002B. This material is widely used in many branches of the industry (automotive, construction, pipeline, etc.) due to its high strength to ductility ratio resulting from a synergetic effect of various strengthening mechanisms. Additionally, precipitation and solid solution strengthened alloys can be processed by SPD much longer than pure metals (due to increased strain hardening rate [34,36]), what is clearly beneficial for the present investigations. Its initial as-received microstructure consisted of a polygonal ferrite structure with the average grain size of about 25 μm. Specimens for the MaxStrain testing were machined out of as-hot rolled plate in the rolling direction – they were 27 mm long and had square 10 × 10 mm cross-sections. During the deformation, total accumulative strains of 2, 5, 7, 10 and 20 were applied. As it was already mentioned, one cycle of MaxStrain deformation consists of two compressive deformations in the state of plane strain, in which two axes are replaced while the longitudinal axis is constrained. Tensile strains are replaced by compressive strains and vice versa. Then, the specimen after each cycle returns to the initial sizes, but the material accumulates strain. Each deformation was fulfilled with the strain $\varepsilon = 0.5$, then, the total accumulative strain after one cycle was $\varepsilon = 1.0$. The dimensions of the cross-section in the middle of the cycle became 16.48 mm × 6.06 mm and after full one cycle they are back to 10 mm × 10 mm. In the present work, specimens were deformed at the room temperature ($T_D = 20$ °C), and then, after the deformation, annealed at the temperature of $T_A = 500$ °C for $t_A = 1200$ s in order to stabilize already obtained UFG microstructure.

After the deformation and heat treatment, the specimens after the second, fifth, seventh, tenth, fifteenth and twentieth cycles were cut and their microstructure was studied using a Scanning