NUMERICAL INVESTIGATION OF THE STATIC RECRYSTALLIZATION INHOMOGENEITIES ACROSS THE PLATE THICKNESS DURING CONTINUOUS ANNEALING

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Abstract

Analysis of static recrystallization inhomogeneities along the thickness of the cold rolled ferritic-pearlitic steel during continuous annealing process is the main goal of the present paper. The multiscale concurrent Cellular Automata Final Element (CAFE) model is used during the numerical investigation. The general concept of the CA algorithm of static recrystallization phenomenon is evaluated. The multiscale model of cold rolling based on the digital material representation (DMR) concept is used to accurately predict deformation energy distribution along the microstructure features and provide input data for the CA model. The final material morphology and recrystallization volume fractions after recrystallization in different plate locations: near the surface, in the middle of a plate, respectively, are evaluated. Finally, examples of obtained results of recrystallized microstructures are compared with the experimental data, to validate the approach.

Key words: cellular automata, static recrystallization, cold rolling

1. INTRODUCTION

The automotive industry focusing on mass car production has great expectations regarding development of new metallic materials with exceptional properties for application in the car body/chassis. This is recently one of the major driving forces of innovative experimental and numerical research in metallurgy and material science institutes across the world. As a result, dynamic development of modern steel grades e.g. Dual Phase (DP) steels has been observed during recent years.

It is estimated that modern car body will contain around 200kg of components made from DP steels by the end of 2020, in comparison to the present level of 60kg (Gorecki et al. 2014). The DP steel contains approx. 70-90% of soft ferrite matrix and 10-30% of hard constituent phase islands. As a result of such complex type microstructure they are characterized by combination of high strength, good formability, high bake hardenability and crash worthiness. DP microstructures are obtained during the continuous annealing process composed of heating of cold rolled steel sheets to the intercritical ferrite-austenite ($\alpha+\gamma$) two-phase region, followed by two-stage or three-stage controlled cooling (Bayram et al., 1999). Due to this complexity, experimental design of the process is time consuming and expensive, thus the development of accurate numerical models that can support mentioned experimental investigations was proposed (Madej et al., 2013; Halder et al., 2014). Present work is focused on numerical modelling of microstructure evolution dur-

ing initial stages of the continuous annealing, namely cold rolling and static recrystallization occurring during heating.

The recrystallization phenomena are usually considered as the two-stage processes: nucleation and grain growth (Humphreys & Hatherly, 1995). After formation of new, strain free, nucleons they start to grow into the deformed matrix at the expense of the stored energy. As a result amount of defects including dislocations in comparison to deformed material is significantly reduced. The most popular numerical approaches to recrystallization that can take microstructure explicitly into account are based on Monte Carlo (MC) and cellular automata (CA) methods (Sieradzki & Madej, 2013). The latter is particularly interesting as major assumptions of this approach can be directly linked to subsequent physical phenomena observed experimentally.

During last few years the CA method has often been applied to model material behaviour under plastic deformation. This includes modelling of static and dynamic recrystallization phenomena (Fei et al., 2014; Popova et al., 2015; Raabe & Hantcherli, 2005; Sitko & Madej, 2014; Ying et al., 2014). The major disadvantage of these approaches was limitation to modelling only micro scale material behaviour. It is well know, that to obtain a detail information on material behaviour, both micro and macro scale material phenomena as well as interactions between them have to be taken into account. The solution to this problem is a combination of micro scale cellular automata model with the multi scale finite element solution – the CAFE (Cellular Automata Finite Element) approach (Seyed Salehi & Serajzadeh, 2012; Sieradzki & Madej, 2012). Thus, the CAFE model was used within the present paper to investigate influence of inhomogenous deformation across the cold rolled plate on static recrystallization behavior during continuous annealing.

2. EXPERIMENT

The experimental material was produce under industrial conditions. The applied rolling reduction was 70%. Simulations of annealing were carried out under laboratory conditions using the dilatometer DIL 805A/D. Samples with chemical composition presented in table 1 and dimension 1mm × 7mm were cut from the centre of the cold rolled sheet parallel to the rolling direction and were heated at a rate of 3°C/s to temperatures in the range 650-775°C. Cooling was carried out in one step to ambi-

ent temperature at rate of 70°C/s. To examine the state of the samples subjected to annealing, the EBSD (Electron Back Scattered Diffraction) analysis was conducted. EBSD patterns were acquired using an acceleration voltage of 20kV. All analysis were conducted on a hexagonal scan grid 180 × 70μm with a scan step size 0.5μm. The EBSD data were post-processed by means of the TSL® software as seen in figure 1.

Table 1. *Chemical composition of analysed material.*

C	Si	Mn	P	S	N	Al	Cr	Nb
0.16	0.39	1,53	0,009	0,002	0,006	0,04	0,23	0,013

In the analysis of the recrystallized fraction, Grain Average Misorientation (GAM) parameter is very useful. It expresses average misorientation between points inside one grain (Kapoor et al., 2009; Radwański, 2015). It is adopted that for recrystallized grains the value of GAM parameter is lower than 0.5°. Results representing maps with marked grains for which GAM≤0.5° are presented in figure 1. As seen the recrystallized fraction is increasing with temperature.

To replicate presented industrial and laboratory experiments a multi scale finite element cold rolling as well as cellular automata static recrystallization models, were used.

3. MULTISCALE FINITE ELEMENT MODEL OF COLD ROLLING

In order to effectively link micro scale cellular automata with the FE simulation the multi scale finite elements model of cold rolling was developed first. It consists of two elements: macro model of cold rolling with regular rectangular mesh figure 2c and micro model based on the digital material representation (DMR) concept, which can take microstructure explicitly into account figure 2a. This approach was developed in (Madej et al., 2013) and proved its advantages in numerical investigation of micro scale heterogeneities.

To investigate differences in strain accumulation across the sheet thickness, and their further influence on SRX, two characteristic locations near the surface and in the center were selected as case studies (figure 2b). The digital material morphology was recreated on the basis of image analysis techniques applied to optical microscopy pictures as seen in figure 2a. Based on the morphology a conforming mesh
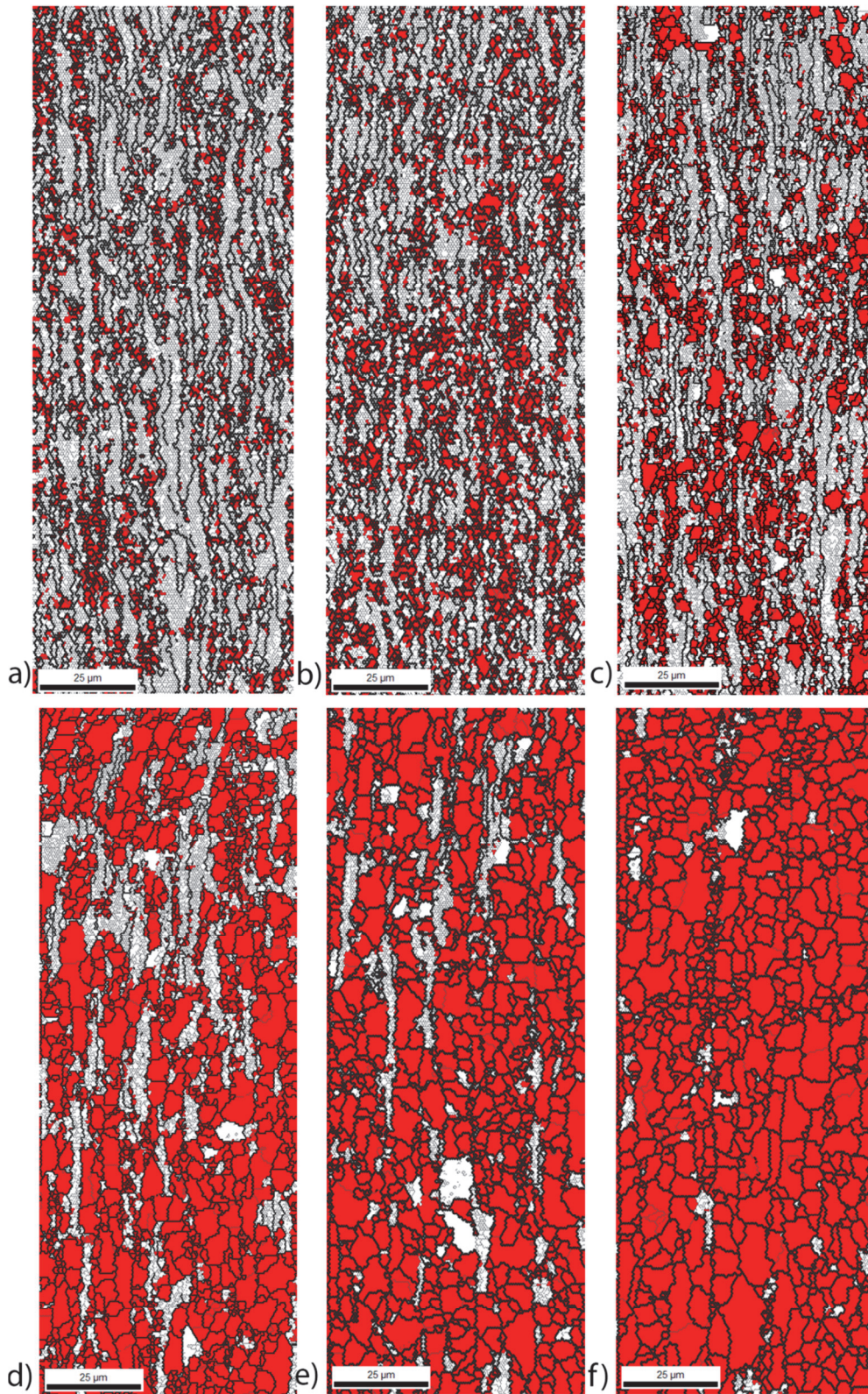
Fig. 1. Maps with highlighted grains of the value of parameter GAM≤0.5° considered as recrystallized ones after annealing the samples at the following temperatures: a) 650°C, b) 675°C, c) 700°C, d) 725°C, e) 750°C, f) 775°C.

that exactly replicates phase and grain boundaries was generated using the *DMRmesh* software (Madej et al., 2011). To minimize computation time, the generated mesh was refined only along grain/phase boundaries. Finally, selected flow curves describing subsequent phases of ferrite and pearlite, respectively, were assigned to particular grains in the microstructure (Madej et al., 2013). The developed model
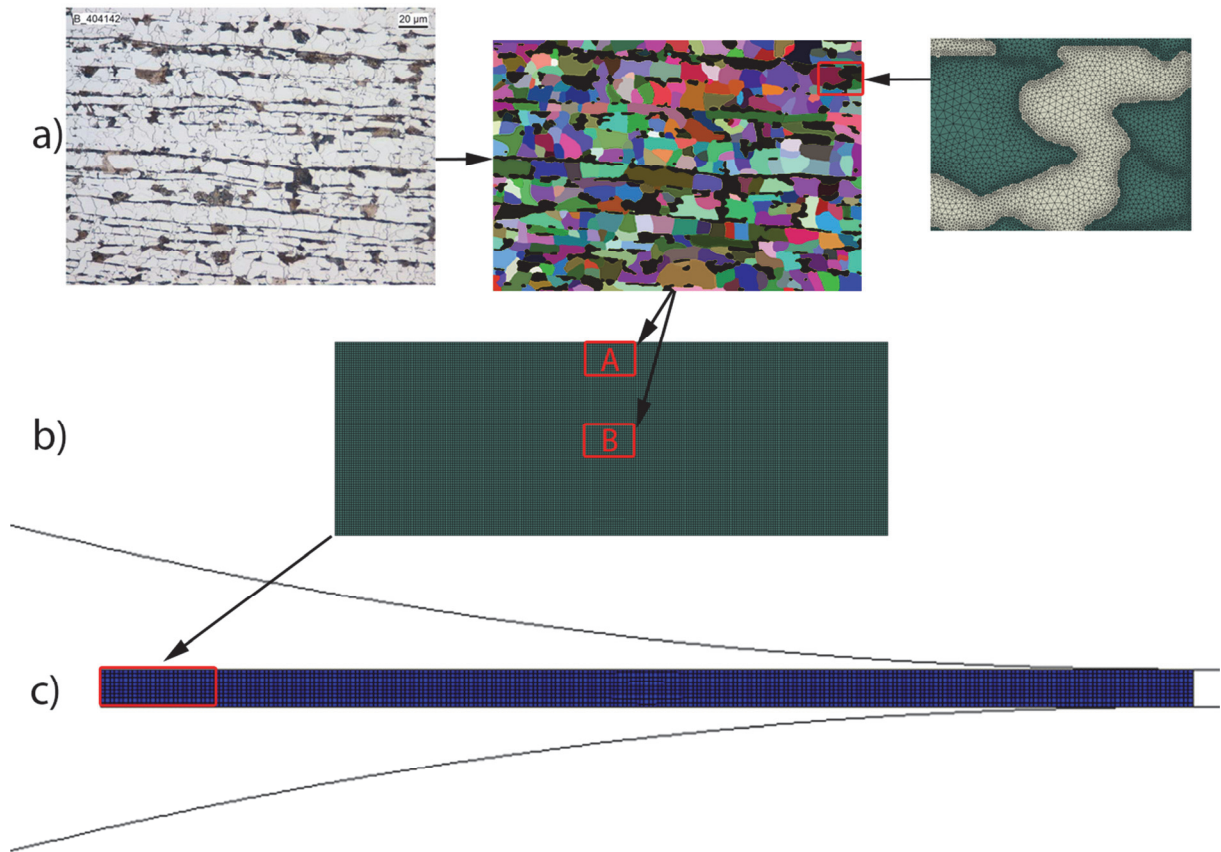
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Fig. 2. *Concept of the multi scale finite element model: a) digital material representation with conforming mesh, b) position of DMRs in the sheet: A (surface) and B (centre), c) macro scale model of cold rolling.*
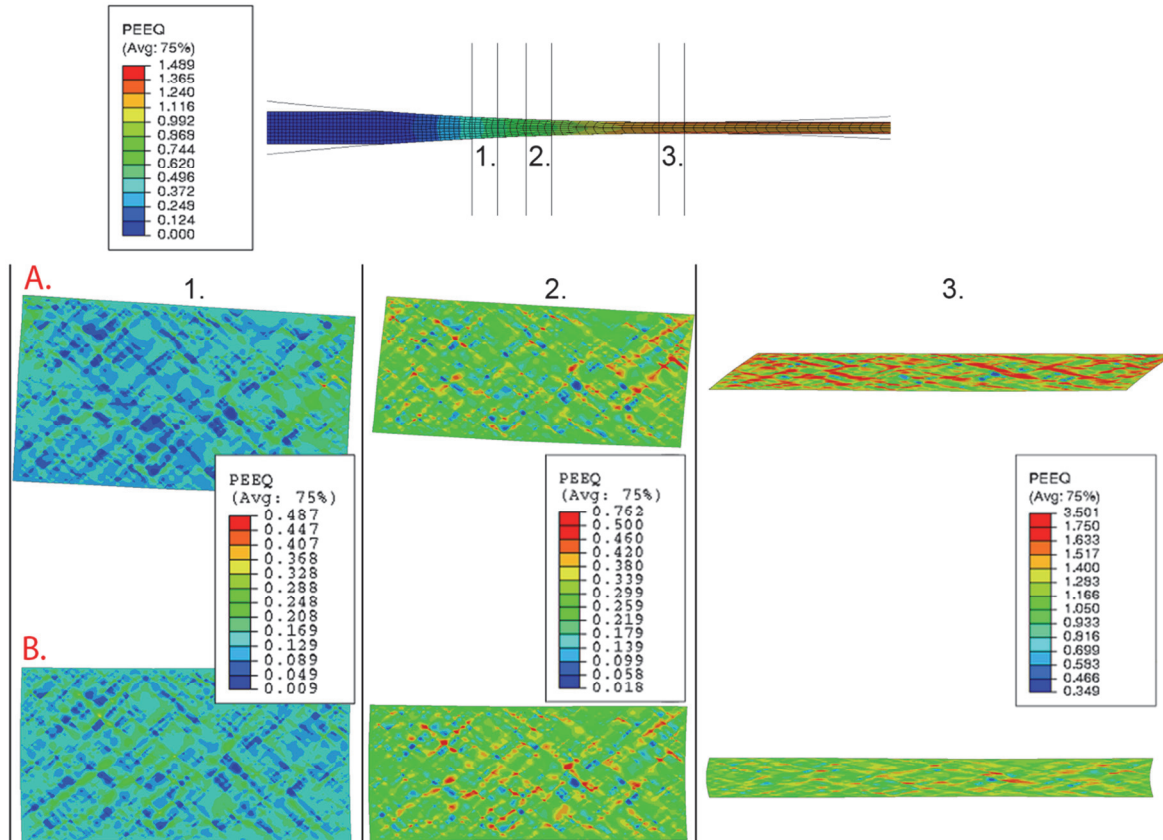

Fig. 3. *Equivalents strain at different stages of deformation.*

was simulated using the commercial finite element software Abaqus.

Obtained results in the form of equivalent strain distributions both at macro as well as micro scale levels are presented in figure 3.

Obtained information on microstructure morphologies as well as stored energy of plastic deformation after cold rolling were then an input data for the micro scale cellular automata model of static recrystallization.

4. CELLULAR AUTOMATA STATIC RECRYSTALLIZATION MODEL

The general concept and assumption of the CA technique to simulation of grain growth and static recrystallization can be found in previous authors work (Madej et al., 2013). Thus, only most important elements of the model and its recent extensions are presented below.

The developed SRX CA model is generally composed of the tree main steps: preparation of initial microstructure, nucleation of new grains and finally, grain growth.

During the first stage, the primary microstructure is preprocessed in order to transfer it into the digital material representation (DMR) form (Madej et al., 2013).

The nucleation in the CA model is based on physical rules and takes into account the influence of physical temperature. The number of nuclei that can appear in the material volume per unit of time is controlled by the equation:

$$N = M_N \exp\left(-\frac{Q_a}{RT}\right), \qquad (1)$$

where: Q_a – activation energy for nucleation, R – universal gas constant, T – temperature, M_N – coefficient computed using the formula:

$$M_N = C_0(H_i - H^C), \qquad (2)$$

where: C_0 - scaling parameter, H_i - amount of energy in the particular cell obtain from deformation in Abaqus software (Madej et al., 2011), H^C - critical amount of energy, which is necessary to trigger nucleation.

H^C is calculated from the formula:

$$H^C = \frac{\varepsilon_c}{a\varepsilon_c + b}\gamma_{lagb}, \qquad (3)$$

where: ε_c – critical plastic strain, a, b – parameters, which are fitted during the experimental analysis, γ_{lagb} - low angle grain boundary energy.

The probability of nucleation in the unit of time is computed as:

$$P_n = NS_N t_{step}, \qquad (4)$$

where: S_N – the volume in which the nucleus can appear, t_{step} – the length of time step in each CA iteration.

Influence of the recovery process on the amount of accumulated energy is considered in the present research and results in lower value of the accumulated energy in particular cells:

$$H_i = \left[H_{i0}^{1/2} - C_1\mu^{-1/2}kT\ln\left(1+\frac{t}{\tau_0}\right)\right]^2, \quad (5)$$

where H_{i0} – the initial stored energy density from deformation, C_1 – a fitting parameter, k – the Boltzmann constant, τ_0 – time constant which is set as 1s, t – time.

The kinetics of the growing nuclei is described by the standard equation:

$$v_k = MP, \qquad (6)$$

where: M - grain boundary mobility, P - net pressure on the grain boundary.

The value of M was computed as:

$$M = \frac{D_0 b_B{}^2}{kT}\exp\left(-\frac{Q_b}{RT}\right), \qquad (7)$$

where: D_0 – diffusion constant, b_B – Burger's vector, Q_b – activation energy for grain boundary motion.

The value P on the other hand was calculated from the following formula, that also considers the pinning force from precipitates:

$$P = H_i + \left(-\frac{3}{2}\gamma_{lagb}\frac{f}{r}\right), \qquad (8)$$

where: f – the volume fraction of spherical particles, r – the particle radius.

The level of coverage of the particular cell by the recrystallization front in the t-th time step was computed by:

$$RX_{i,j,t}^{fraction} = RX_{i,j,t-1}^{fraction} + \sum_{k=1}^{rx}\left(\frac{v_k t_{step}}{c_s}\right), \qquad (9)$$

where: $RX_{i,j,t-1}^{fraction}$ – the level of coverage in the t-1-th time step, rx – number of recrystallized neighbors (stored energy driving force), v_k - velocity of the recrystallization front (6).

Thus, based on the above equations a governing transition rule describing changes in the unrecrystallized ($uSRX$) to recrystallized (SRX) state is defined as:

$$Y_{i,j,t+1} = \begin{cases} SRX \Leftrightarrow RX_{i,j,t}^{fraction} > 1.0 \\ Y_{i,j,t} \end{cases}, \qquad (10)$$

where: $Y_{i,j,t}$ – state of the neighboring cell (i,j) in a particular time step t.

5. RESULTS

As mentioned, results from the FE cold rolling performed in Abaqus software were used as input for the described cellular automata code. Deformed microstructure morphologies were transferred into the CA space as image pixels, while accumulated energy values were interpolated using interpolation methods (Madej et al., 2013). Parameters used during the SRX simulation are collected in table 2.

Samples were heated with constant heating rate of 3 °C/s up to different temperatures and obtained microstructure morphologies were investigated (blue and green color represent primary grains, red color
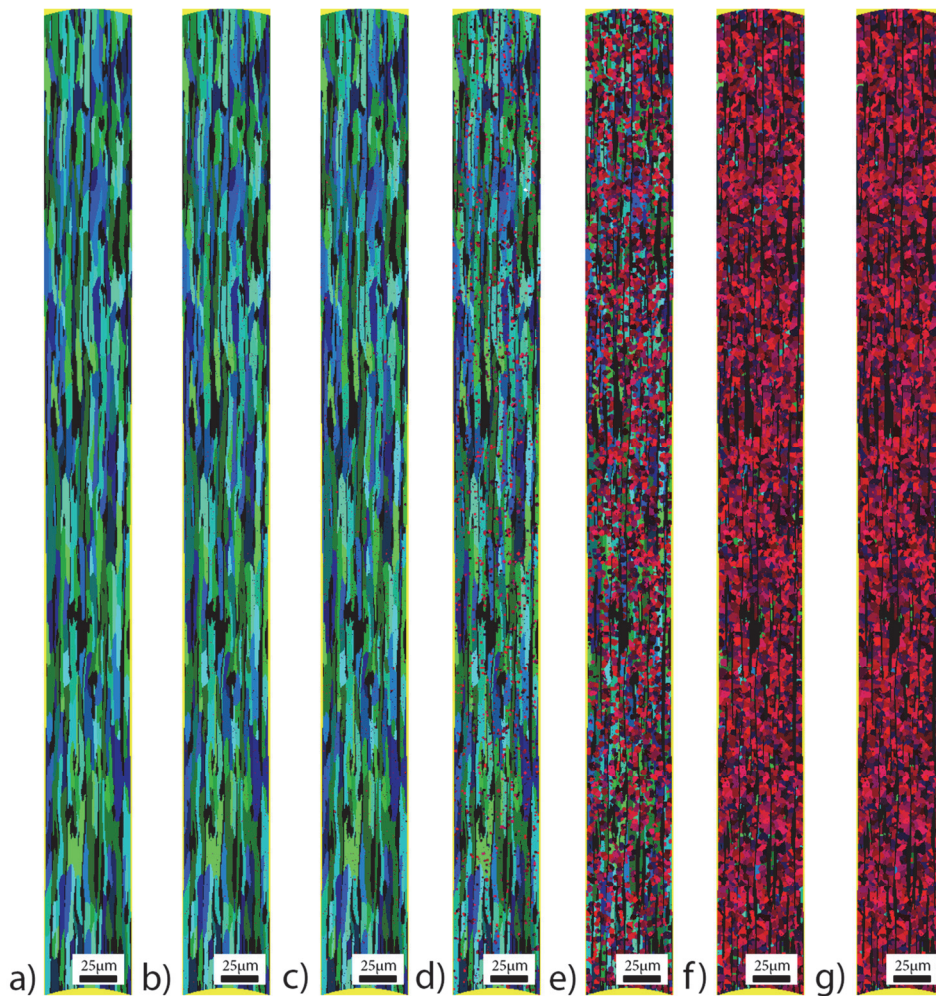

Fig. 4. Evolution of microstructure (figure 2 region B) during static recrystallization with heating rate 3°C/s at different temperatures a) room, b) 650°C, c) 675°C, d) 700°C, e) 725°C, f) 750°C, g) 775°C.

Table 2. Parameters used in the SRX simulation.

Q_a	C_0	C_1	a	b	D_0	b_B	r	t_{step}
146 kJ/mol	0.55	1e26	1.8e-9	0.9e-7	1.1e-6 m²/s	2.48e-10	0.05e-6m	0.1
ρ	γ_{HAGB} -	A	$c_{s\ middle}$	$c_{s\ top}$	Q_b	γ_{lagb}	G	f
8.8e14 m⁻²	0.56 J/m²	1.28	0.55e-6 m	0.57e-6 m	155 kJ/mol	0.2 J/m²	5,97e10 Pa	0.01

represent recrystallized grains). Microstructure presented in figure 4 was located in the center of the cold rolled sheet, while results for the microstructure near the surface are gathered in figure 5.

5. CONCLUSIONS

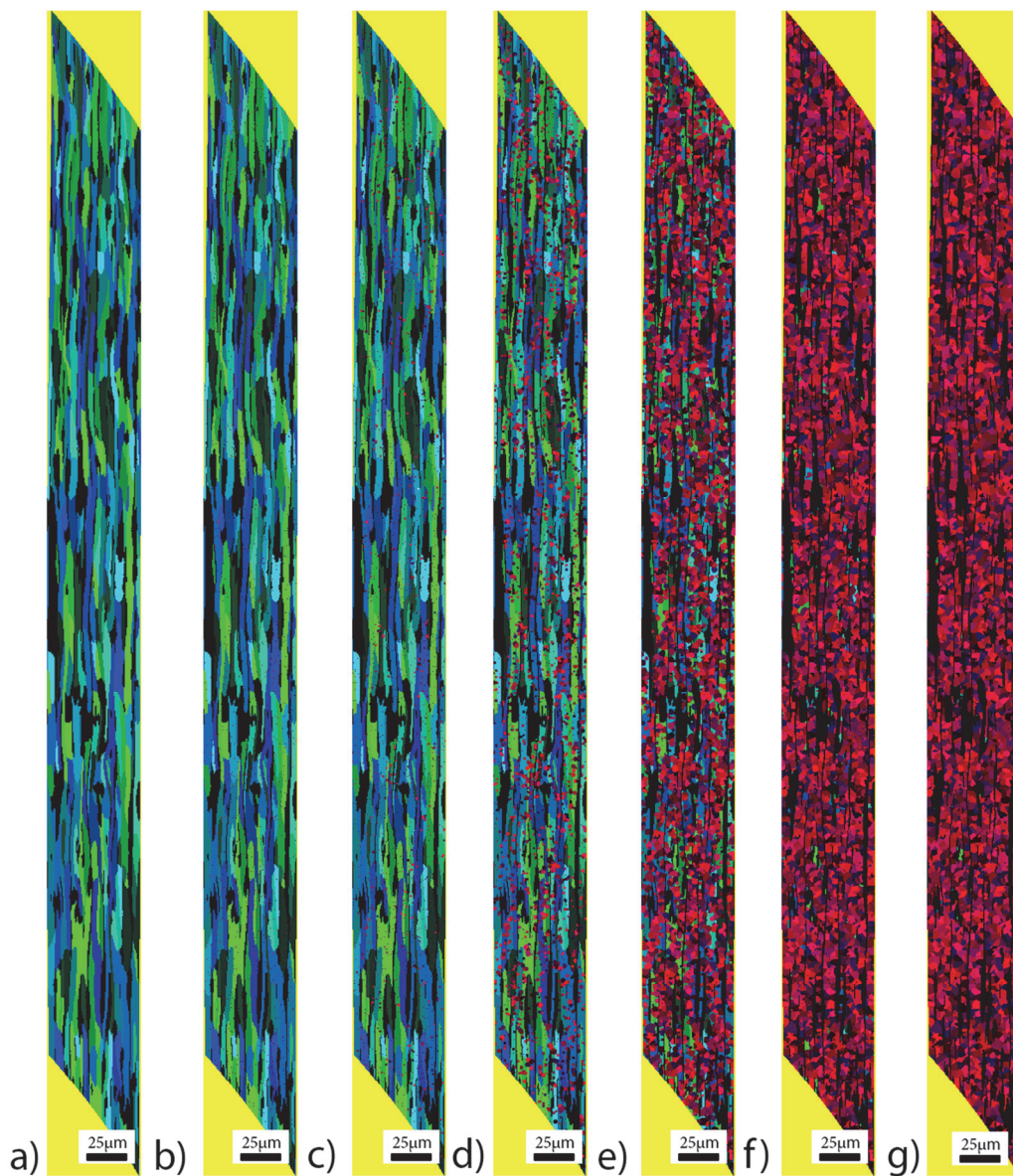Following conclusions can be drawn based on the presented results,

Fig. 5. Evolution of microstructure (figure 2 region A) during static recrystallization with heating rate 3°C/s at different temperatures a) room, b) 650°C, c) 675°C, d) 700°C, e) 725°C, f) 750°C, g) 775°C.

Quantitative comparison of final grain size as well as recrystallization kinetics are shown in figure 6.

As seen the inhomogeneities in strain distribution across the cold rolled plate influence the static recrystallization kinetics. However, when final grain size is considered the influence is moderate. The final grain size is approx. 2.5 μm in both cases, and it agrees with experimental measurements.

As seen obtained experimental results confirm good predictive capabilities of the developed numerical CAFE model, which can be used to investigate various heating conditions used by industry.

- The multi scale concurrent digital material representation finite element model is an efficient solution to investigate heterogeneities at the micro scale level and to provide input data for the cellular automata technique.
- The DMR models can be applied to investigate influence of deformation conditions on accumulated energy levels.
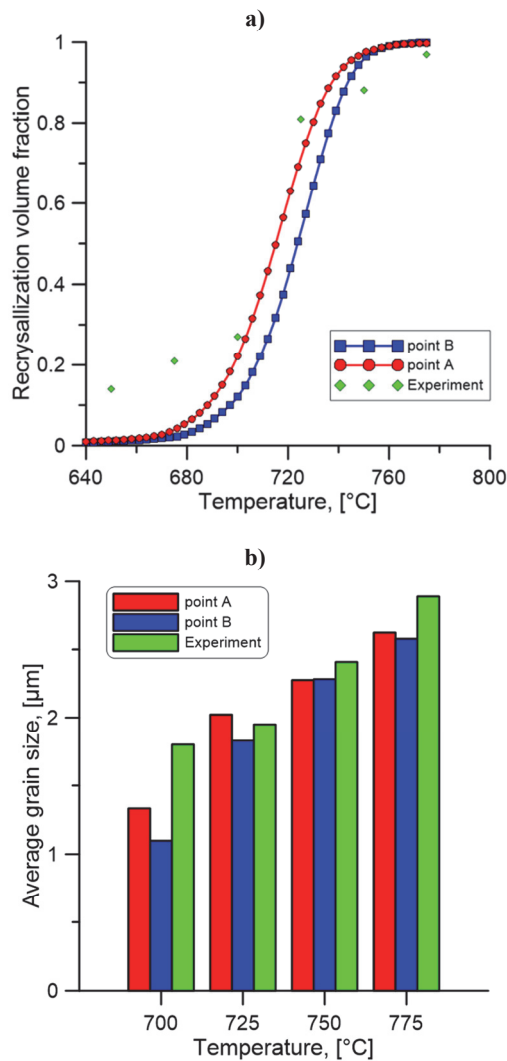
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Fig. 6. Comparison of a) recrystallization volume fraction, and b) grain sizes.

- Good predictive capabilities of the CA model were confirmed by the industrial cold rolling and laboratory static recrystallization measurements.
- Combination of the finite element and cellular automata models provides a possibility to predict inhomogeneities in the sheet properties during the continuous annealing process.

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REFERENCES

Bayram, A., Uguz, A., Ula, M., 1999, Effects of microstructure and notches on the mechanical properties of dual-phase steels, *Materials Characterization*, 43, 259-269.

Fei, C. , Ke, Q. , Zhenshan, C. , Xinmin, L., 2014, Modeling the dynamic recrystallization in austenitic stainless steel using cellular automaton method, *Computational Materials Science*, 83, 331-340.

Gorecki, G., Madej, L., Pietrzyk, M., 2014, Computer system for the design of optimal thermal cycles in the continuous annealing of DP steels, *Journal of Machine Engineering*, 1, 74-83.

Halder, C., Madej, L., Pietrzyk, M., 2014, Discrete micro-scale cellular automata model for modelling phase transformation during heating of dual phase steels, *Archives of Civil and Mechanical Engineering*, 14, 96-103.

Humphreys, F.J., Hatherly, M., 1995, *Recrystallization and Related Annealing Phenomena*, Elsevier.

Kapoor, R., Paul, B., Raveendra, S., Samajdar, I., Chakravartty, J.K., 2009, *Metallurgical and Materials Transactions A*, 40A, 818.

Madej, L., Rauch, L., Perzyński, K., Cybułka, P., 2011, Digital Material Representation as an efficient tool for strain inhomogeneities analysis at the micro scale level, *Archives of Civil and Mechanical Engineering*, 11, 661-679.

Madej, L., Sieradzki, L., Sitko, M., Perzyński, K., Radwański, K., Kuziak, R., 2013, Multi scale cellular automata and finite element based model for cold deformation and annealing of a ferritic-pearlitic microstructure, *Computational Materials Science*, 77, 172-181

Madej, L., Szyndler, J., 2013, Effect of number of grains and boundary conditions on digital material representation deformation under plane strain, *Archives of Civil and Mechanical Engineering*, 14, 360-369.

Popova, E., Staraselski, Y., Brahme, A., Mishra, R.K., Inal, K., 2015, Coupled crystal plasticity – Probabilistic cellular automata approach to model dynamic recrystallization in magnesium alloys, *International Journal of Plasticity*, 66, 85-102.

Raabe, D., Hantcherli, L., 2005, 2D cellular automaton simulation of the recrystallization texture of an IF sheet steel under consideration of Zener pinning, *Computational Materials Science,* 34, 299-313.

Radwański, K., 2015, Application of FEG-SEM and EBSD methods for the analysis of the restoration processes occurring during continuous annealing of Dual-Phase steel strips, *Steel Research International*, DOI: 10.1002/srin.201400361.

Seyed Salehi, M., Serajzadeh, S., 2012, Simulation of static recrystallization in non-isothermal annealing using a coupled cellular automata and finite element model, *Computational Materials Science,* 53, 145-152.

Sieradzki, L., Madej, L., 2012, Modeling of the static recrystallization with cellular automata method and digital material representation approach, *Metal Forming 2012: proceedings of the 14th international conference on Metal Forming: Steel Research International; spec. ed.,* 1139-1142.

Sieradzki, L., Madej, L., 2013, A perceptive comparison of the cellular automata and Monte Carlo techniques in application to static recrystallization modeling in polycrystalline materials, *Computational Materials Science*, 67, 156-173.

Sitko, M., Madej, L., 2014, Development of dynamic recrystal-lization model based on Cellular Automata approach, *Key Engineering Materials*, 622-623, 617-624.

Ying, Z., Xianghua, L., Hailiang, Y., 2014, Cellular automaton simulation of hot deformation of TRIP steel, *Computational Materials Science*, 81, 104-112.

ANALIZA NUMERYCZNA NIEJEDNORODNOŚCI ROZWOJU MIKROSTRUKTURY NA GRUBOŚCI PASMA PODCZAS CIĄGŁEGO WYŻARZANIA

Streszczenie

Celem niniejszej pracy jest analiza numeryczna niejednorodności rozwoju mikrostruktury na grubości pasma stali ferrytyczno-perlitycznej podczas ciągłego wyżarzania. W pracy wykorzystano współbieżny model wieloskalowy na bazie metody elementów skończonych połączonej z metodą automatów komórkowych (Cellular Automata Final Element - CAFE). Model wieloskalowy walcowania na zimno oparto na idei cyfrowej reprezentacji materiału do dokładnego określenia energii zmagazynowanej w materiale w wyniku odkształcenia plastycznego, która zostanie wykorzystana jako jeden z parametrów początkowych modelu automatów komórkowych. Następnie przedstawiono wyniki w postaci morfologii materiału wraz z odpowiadającymi ułamkami części zrekrystalizowanej po procesie nagrzewania odpowiednio: przy powierzchni oraz w środku płyty. Uzyskane wyniki obliczeń numerycznych zostały porównane z danami eksperymentalnymi w celu walidacji modelu.