Comparison between experimental data and a cellular automata simulation of martensite formation during cooling

A Kaijalainen, O Seppälä, V Javaheri, A Pohjonen, D Porter and J Kömi
Materials and Mechanical Engineering, Centre for Advanced Steels Research, University of Oulu, Oulu, Finland

Corresponding author email: antti.kaijalainen@oulu.fi

Abstract. Computer simulations of steel microstructural development provide a powerful tool, which can form the basis of mechanical property predictions. However, in order to create detailed understanding of the factors affecting the properties, the model should predict microstructural evolution during cooling. The present study compares the results of cellular automata simulations with experimental data for two distinct austenite conditions, recrystallized and deformed. Detailed microstructural features were studied using a laser scanning confocal microscope, FESEM and FESEM-EBSD. The two-dimensional cellular automata (CA) model for simulating the formation of lath martensite was parameterized using fitted Johnson-Mehl-Avrami-Kolmogorov and Koistinen-Marburger equations. The parent austenite microstructure for the CA model was determined from the final martensitic microstructure using austenite grain reconstructions based on the use of MATLAB software and the MTEX toolbox. The results of this cellular automata simulation can be used to estimate the shapes and sizes of martensite blocks, which offers new possibilities for the qualitative estimation of the mechanical properties of high-strength steels formed from recrystallized or deformed austenite.

1. Introduction
The development of novel ultra-high strength steels (UHSS) requires metallurgical knowledge together with much experimentation. Especially, for direct-quenched steels, where the cooling process after the last hot rolling pass dictates the final mechanical properties, a good understanding of on-cooling phase transformation is needed [1]. Achieving a fully martensitic microstructure is the key factor for having high strength and high toughness in these steel grades [2]. However, the process parameters along with the chemical composition affect the phase transformations and thus the microstructure. The evolution of microstructure with the aid of cellular automata (CA) has been studied by several authors [3–6]. CA has been successfully used to simulate the recrystallization and grain growth of steel by Sieradzki and Madej [3] and annealing following cold deformation by Madej et al. [4]. Also, austenite-ferrite phase transformations and the resulting carbon diffusion during isothermal heating and continuous cooling have been simulated by An et al. [5] and austenite-ferrite-pearlite transformations during the thermal cycle of dual-phase steel by Bos et al. [6]. The current study employs the model of Seppälä et al. [7], a novel CA method used to simulate bainite and martensite transformation. The model is based on the well-established Koistinen-Marburger (K-M) equation [8].

Prior austenite state and grain size also plays a crucial role regarding the final microstructure. Hence, to evaluate and to estimate the on-cooling phase transformations, the prior austenite grain structure
should also be taken into consideration. To reveal the prior austenite grain structure, a reconstruction method is commonly used for martensitic and bainitic microstructures that have been formed from equiaxed [9,10] and highly pancaked prior austenite [11,12] with a Kurdjumov–Sachs orientation relationship (K–S OR) [13]. In the near future, microstructural computation will be a powerful tool able to reduce the amount of experimental work needed in steel development. The novel CA model for simulating the formation of martensite in steels is one step towards this objective. The aim of this study is the verification of the CA simulation proposed in [7] for martensite formation with the help of experimental EBSD data.

2. Experimental material and methods

2.1. Thermomechanical treatments and material characterization

The studied steel composition in wt.% was 0.14C-0.2Si-1.1Mn-0.7Cr-0.2Mo-0.03Ti-0.002B. Dilatation data for recrystallized and pancaked austenite were obtained using a Gleeble 3800 thermomechanical simulator. Cylindrical samples made from the steel were initially solution treated at 1250 °C for 2 hours followed by water quenching. The specimens were subsequently heated at 10 °C/s to 1100 °C, held for 2 min, cooled to 1050 °C or 850 °C, held 15 s, and then compressed with three hits each having a strain of ~0.2 at a strain rate of 1/s. Then the specimens were held 5 s before cooling at 70 °C/s. This gave two distinct austenite conditions: one recrystallized (1050 °C) and the other pancaked (850 °C) for comparison with the CA simulations. A general characterization of the transformation microstructures was performed with a field emission scanning electron microscope (FESEM) (Sigma, Zeiss) on specimens etched with nital.

Electron backscatter diffraction (EBSD) measurements and analysis were performed using the EDAX-TSL 7.0 acquisition and analysis software. The FESEM for the EBSD measurements was operated at 15 kV with a step size of 0.15 µm when studying areas ~110 x 110 µm and 0.4 µm for the larger area ~220 x 220 µm. Samples were subsequently re-polished to remove the contaminated layer after EBSD and the prior austenite grain structure was investigated using a laser scanning confocal microscope (LSCM) after picric acid etching from the same area.

2.2. Parent austenite reconstruction method

In order to have a good initial assumption of the parent austenite grain structure for the CA simulations, the parent austenite grain structure was revealed using a reconstruction technique. The EBSD data of the dilatometry samples were subjected to the reconstruction using Matlab software supplemented with the MTEX texture and crystallography analysis toolbox [14]. Initially, grain maps were created from the data sets with a grain boundary tolerance of 3-5 degrees. Then, the parent austenite orientation map was reconstructed from the assembled grain maps with a two-step reconstruction algorithm. In the first step of the process, the orientation relationship between austenite and martensite was determined using K-S orientation relationship i.e. {111}//{110}, <110>//<111>, where there are 4 {111} planes which are parallel to a {110} plane and each {111} plane contains 3 <110> directions, each of which is parallel to 2 <111> directions. Consequently, 24 different crystallographic variants of the bcc structure (bainite/martensite) can form within one former fcc (parent austenite) grain. According to Morito et al. [15], the 24 variants generated by the K-S OR are categorized into four packet groups. In a packet, all variants share the same close-packed planes. Each packet then contains six variants depending on the parallel directions. Although the exact parallelism of planes and directions of the K-S orientation relation cannot be observed in actual crystallographic measurements of martensite, the consistent variant labeling system by Morito et al. [15] has been used to successfully identify a number of martensitic/bainitic microstructures with varying orientation relationships between the fcc and bcc structures. Afterwards, in the second step, the grain map was divided into distinct clusters using the Markov clustering method [16] proposed by Gomes and Kestens [17]. The parent austenite orientation was then calculated for each cluster separately, resulting in a reconstructed orientation map. The average misorientation between the reconstructed orientation for each cluster and the best fit for each individual
grain was approximately 2 degrees, indicating a good fit for the reconstructed result. The full details for the reconstructed procedure are available in Ref. [18].

2.3. **Cellular automata algorithm**

Cellular automata [19] is a method in which the modelled area is divided into equal-sized elements, i.e. cells. These cells have various properties which can be altered by a user-defined set of rules. In this case the only property needed for a cell is a color code that defines its current phase and separates instances of the same phase divided from each other by a high-angle grain boundary. Each cell represents a finite area of a single phase and several adjacent cells with the same color code represent a single grain (austenite) or block (martensite).

The CA-algorithm used in the current study starts from a situation where the microstructure is fully austenitic. At the end of every step the output created by the simulation is saved and an end condition check is performed. If end condition requirements are satisfied the simulation ends, otherwise it continues. Algorithms calculate the amount of new martensite nuclei and their growth speeds. As the simulation advances, new nuclei are placed into the simulation area and start growing with respect to their growth rules. Lath martensite grows as blocks, which consist of thin disc-like laths which grow next to each other. A single lath grows lengthwise at a very high speed with a constant width. The lath grows until it collides with a high-angle grain boundary. Widthwise growth of a block occurs gradually as new nuclei appear next to an existing block and grow in the same direction, adding to the width of a block [20].

3. **Results and discussion**

Figures 1-4 illustrate the microstructures of samples strained at 1050 °C (recrystallized) and 850 °C (pancaked) with two acquisition areas including EBSD image quality (IQ) maps with high-angle grain boundaries (HAGB, >15°), i.e. prior austenite, block and packet boundaries (figures 1-4a). A smaller area with a finer step size can produce better IQ and therefore more detailed grain size information. However, only few prior austenite grains are covered in the 110 x 110 µm area (figures 1a and 3a). Thus, a larger area (220 x 220 µm) was also examined, producing quantitative data of prior austenite grains, which are reconstructed with Matlab MTEX code as can be seen in figures 2b and 4b. In the CA simulated images (figures 1-4c), the black lines are parent austenite grain boundaries from the MTEX reconstructions and red tones are martensite blocks with their boundaries as blue lines. MTEX reconstructed parent grains were used as the initial austenitic microstructure in the CA simulations. MTEX reconstructed, recrystallized parent austenite grains were found to match extremely well with the picral etched optical microscope images even though a thin layer was polished away after the EBSD acquisitions. In the pancaked austenite, the grain boundaries are not so clear since some new small grains have nucleated on the grain boundaries after strain at 850 °C. For this reason, the MTEX reconstruction does not work as well as with equiaxed grains, but the information is still suitable for the CA simulations.

The EBSD grain sizes were determined using the equivalent circle diameters (ECD) of grains surrounded by HAGB. CA simulations show block boundaries. Grain size distributions and area fractions of the experimental data with two levels of data clean-up together with the CA simulations are shown in figures 5-6. The CA simulations are done with a 1 µm step size to prevent formation of artefacts during the simulations and the finest ECD grain size is ~1.13 µm. EBSD ECD grain size distributions, also filtered to remove grains smaller than ~1.0 µm, are comparable to those obtained from the CA simulations. In both cases mean ECD grain sizes are at the same level. However, there are more differences when comparing the area fractions. A few large grains might be artefacts due to undetected grain boundaries in the EBSD acquisitions. Nevertheless, experimental and simulated grain sizes and morphologies are seen to correspond well for the martensitic microstructures studied.
Figure 1. 3×0.2 strain at 1050 °C, small scanned area. (a) Original EBSD image quality map with high-angle boundaries (HAGB, >15°, blue), (b) MTEX reconstructed prior austenite grains, (c) CA simulated martensite blocks (red) with block boundaries (BB, blue) and (d) prior austenite grain boundaries after picral etching.

Figure 2. 3×0.2 strain at 1050 °C, large area. (a) Original EBSD image quality map with high-angle boundaries (HAGB, >15°, blue), (b) MTEX reconstructed prior austenite grains, (c) CA simulated martensite blocks (red) with block boundaries (BB, blue) and (d) prior austenite grain boundaries after picral etching.

Figure 3. 3×0.2 strain at 850 °C, small area. (a) Original EBSD image quality map with high-angle boundaries (HAGB, >15°, blue), (b) MTEX reconstructed prior austenite grains, (c) CA simulated martensite blocks (red) with block boundaries (BB, blue) and (d) prior austenite grain boundaries after picral etching.

Figure 4. 3×0.2 strain at 850 °C, large area. (a) Original EBSD image quality map with high-angle boundaries (HAGB, >15°, blue), (b) MTEX reconstructed prior austenite grains, (c) CA simulated martensite blocks (red) with block boundaries (BB, blue) and (d) prior austenite grain boundaries after picral etching.
4. Conclusions
The aim of this study was to verify a detailed model for martensite transformations by using a novel cellular automaton that simulates martensite transformation graphically in a given austenite grain structure. The simulation results need to be linked to a certain material to make them comparable to real life. The simulation and experimental results were compared by analyzing microstructural images and grain sizes. The shape and size of martensite blocks was found to be in good correspondence when similar grain size filtering was used.

In its current form, the CA simulation can be used to simulate the resulting morphology of the martensite blocks in the thermomechanically processed steel in question to a higher degree of detail than is possible using the macroscopic K-M model. The detailed morphology can be used to estimate the mechanical properties of the steel and it could also be used as input information into other simulation tools, for example fatigue models. Hopefully, in the future, the orientations of austenite grains can be
implemented into the CA model to produce the texture of the transformed bcc phase on the basis of a K-S orientation relationship as in authors’ previous study [11].

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