Simulation of hot rolling by cellular automata

T Hegyes¹ and P Barkóczy²

¹ Arconic Köfém Mill Products Hungary Kft., Székesfehérvár, Hungary
² Fux Zrt., Miskolc, Hungary

E-mail: tibor.hegyes@arconic.com

Abstract. This development is focusing on one of the most complex and important production steps of flat rolled products that is the simulation of hot rolling. During hot rolling two phenomena, work hardening and the process of regeneration of microstructure have strong influence for physical properties of aluminium alloys. Dynamic recovery has importance in the dynamic softening beside dynamic recrystallization in aluminium alloys. Hot rolled and newly modified grain structure is influenced by these dynamic phenomena. Hot rolled grain structure goes through significant changes under further production steps like cold rolling and heat treatments. But aside from these intermediate production steps the microstructure that we get after hot rolling has significant effect on mechanical and grains structure of the final flat rolled product. Proper cellular automata simulations of recrystallization and recovery can be the basis for good technology planning practices.

1. Introduction

Worldwide, millions of tons of flat rolled aluminium sheets are produced per year for customers. For a technology engineer it is not an easy task to build up a proper technology that fulfils the product requirements. These requirements that we can call material properties like material thickness, grain size, mechanical properties, deep drawing capability etc. are in focus for end users and the rolled material must conform to these specified customer requests [1]. Therefore, a development of a simulation has an importance that could support industrial engineers in their daily practice to find the best optional production route. One possibility is to simulate the whole production process [2], but at first hand the simulation of material behaviour and not the technology itself is useful [3]. For the rolling technology simulation from material workability, rolling passes etc. FEM simulations are more common solutions [4]. But when the calculation of the microstructural parameters is important, e.g. deep drawing, it needs to extend to other calculation or simulation methods [5]. One possible extension is the cellular automata [6]. Cellular automata are different, and they could give better solution for recrystallization simulation [7]. Working with cellular automata is easier and calculation time could be shorter. This is an advantage in the mentioned industrial application where time factor is important and material properties are in focus.

The cellular automata are applied for this simulation task is 3D [8], 2D [9] and 1D [10]. The 3D and 2D simulations give a detailed picture about the development of the microstructure. The large number of the used cells, the resolution of the computation, has a great effect on the computation time. For this aspect the 1D simulations are extremely effective ones, but the mentioned detailed picture is lost. But calculation of the average grain size, and the distribution of grain sizes are easy with these automata.
The automata use arbitrary units during the calculation. Therefore a scaling step is necessary for the evaluation of the calculation [11].

Cellular automata is a discrete dynamic method with a simple calculation scheme. Therefore, the calculated results and parameters have special measures, which derived from the operation of the automata. Such like the time, which measured in automata steps, and the distance which measured by cells. There is no information in the sub-cell region, or no valid states inside a step. These two main measures change the other derived measures of all used parameters. Basically, the automata make the calculation well if the real parameters converted to this specific universe. This conversion called scaling, and method in [11] uses a Nelder-Mead simplex method for the mentioned conversion based on the comparison of measured and calculated results. In this method the time scale, which is the quotient of the real time period and automata steps, is fixed and the kinetic parameters, for example the activation energies of the processes vary by the simplex method.

The [10] automaton is used in the current development. This is a 1D automaton with periodic boundary conditions in both ends of the universe [12]. The periodic boundary condition makes the state of the cells identical at both ends of the universe. This assumption means that the processes take place in the bulk, far from the surface regions. The basic states of the cells are deformed and recrystallized.

The used 1D cellular automaton of recrystallization [7, 10] is used in several study e.g. kinetic analysis of recrystallization of OFHC copper, simulation of crystallographic changes during recrystallization of rolled sheets etc. Only two aspects are missing to apply this automaton to a process simulation: one is the coupling the simulation of recovery to the automaton of recrystallization, and the description of the dynamic recovery and recrystallization in a same way as it used in [7, 10]. This article introduces the solution of these missing calculations to prepare the automaton the process simulation of production of rolled flat sheet products. The key for this is the stored energy as a state variable is used in the description of the states of the cells as in [10]. The different sub-processes changing the value of it. The deformation process increasing the stored energy according to the strain hardening. The recovery and the recrystallization (nucleation and growth) are decreasing the amount of stored energy. These changes are basically described by the kinetics of the processes and ruled by the kinetic constants. The kinetics calculated by the cellular automaton and the activation energies are used to specify the automata as a given material (alloy and state). In this study the behavior of the developed automaton is introduced through a single hot rolling step. The results are discussed and evaluated on the effect of the different kinetic constants. The basic set-up was chosen from prior study of recrystallization of EN AW 3003 [7], based on this calculation were estimated the kinetic constants. It is important to note that these results calculated by estimated constants, not scaled ones.

2. Recovery simulation by 1D cellular automata

The [10] automaton just calculates the changes during a recrystallization process, and it is scaled to OFHC copper [7]. In this case the recovery has no importance but in case of aluminum alloys it is necessary to couple that calculation with a recovery simulation.

The recovery has no significant effect on the deformed microstructure, but the dislocation structure is rearranged. One basic property where it can be evaluated is the stored energy, which is the driving force of the following recovery and the recrystallization. Therefore, the stored energy (\(E_{st}\)) is incorporated into the state of the cells. This incorporation is changing the meaning of the basic states. So, the critical value of the stored energy is defined (\(E_{crit}\)). The cells which have lower stored energy are recrystallized. In the other case, deformed cells have larger (or equal) stored energy. One other limit is defined, which has a strong connection to the recovery process. The analysis of measured kinetic of softening of aluminum alloys [13] shows that the softening by recovery is asymptotically approximated with a value which depends on the degree of deformation and the alloying. This has a strong connection to the subgrain size and structure. The defined limit of stored energy means that value which can be reached by the recovery process only (\(E_{rec}\)).

The developed automaton connects 10000 cells in 1D like a chain. Every cell has two other neighbors with periodic boundary condition. It means that the first and the last cells in the lace (universe) are
connected to each other. The cell chain becomes unending. During the tests the automaton calculates with 1000 calculation steps. The following basic parameters were set for this capability study of recovery: each cell has deformed state (stored energy: 1000 (J/cell); critical stored energy: 100 (J/cell)). The calculations were made under isotherm circumstances (500 °C). It can be demonstrated like a cold rolled material with height dislocation density/stored energy which is annealed. The dislocation movement as well as the recovery are both thermally activated processes. For the calculation of the stored energy of a cell a same stochastic rule is used as in [10]. The activation energy of the recovery (Q_r) is converted to a probability by the Arrhenius function (1). In every step at every updating of the cell states a random number is generated between 0..1. If the generated random number is lower than the calculated probability, the stored energy is changed by the recovery according to (2). This function means an exponential decay of the individual values of the stored energy. Kst is another kinetic constant next to the activation energy. It has the same effect to the calculated kinetics of the recovery, so it is constant value in the current study. The T denotes the temperature and R is the gas constant.

\[ p = \exp\left(\frac{Q_r}{RT}\right) \]  

\[ E_{st}(t + \Delta t, i) = E_{st}(t, i) - \frac{E_{st}(t, i) - E_{str}}{K_{st}} \]  

In this case also true the assumption in the Introduction, that recrystallization kinetics of EN AW 3003 is the basis. But there is no specific calculation till now to the kinetics of recovery alone with 1D automaton. Additionally, the numerical effect to the incorporated kinetic constants are unknown. Therefore, in the following study the automaton’s arbitrary units are used. The total stored energy is calculated as a summary of the stored energies of the cells. In the first calculation the changes of this value are examined. Figure 1. presents the stored energy changing in function of automata calculation steps using different activation energy. Results show us the different value of activation energy has different effect on the stored energy. Increasing activation energy slows the recovery. The value of stored energy didn’t change efficiently in case of 50 (KJ/cell).

![Figure 1](image)

**Figure 1.** Stored energy changing in function of 1D cellular automata calculation steps with different activation energies

In this case we can say the dislocation density remained high and no significant softening take place. The value of Kst is set to 10 for calculation. Critical stored energy is an important parameter. When a cell reaches this value, the cell becomes recrystallized. Activated cells change their own state in this case from formed state to annealed (recovery) state. Lower value of activation energy is causing drastic drop in stored energy during calculation. The nature of 20 (KJ/cell) activation energy curve is exponential that is typical for recovery mechanism.

3. Coupled simulation of recovery and recrystallization by 1D cellular automata
Recovery and recrystallization are responsible for softening mechanism in aluminium alloys. Our goal was to connect the recovery and recrystallization rules in one automaton that can handle both mechanisms parallel in one calculation.

We used almost the same basic parameters like in the previous chapter for recovery $Q_r=20$ (kJ/cell), $E_{st}=1000$ (J/cell), $E_{str}=100$ (J/cell), and $E_{str}=800$ (J/cell). For this calculation 1500 calculation steps and different temperatures (iso and non-isothermal) were applied. The activation energy of nucleation was 60 (kJ/cell) while the activation energy of growth was 40 (kJ/cell). With these values the recrystallization related to the recovery is defined.

Results were similar until approximately 200 calculation steps (Figure 2-3.), there is an intensive drop in stored energy due to recovery. This is that point where recrystallization become a larger effect in softening than recovery. Over 200 calculation steps curves start to separate from each other and there is big difference in stored energy. Stored energy didn’t change significantly at 300 ($°C$). This was a low temperature for recrystallization, but recovery was responsible for softening. Lowest stored energy was calculated at 500 ($°C$) and the recrystallized volume fraction (F) is almost 0,9 after calculation. This is a typical curve of Avrami type phase transformation. In the reality there is non-isothermal cooling therefore we simulated this case also. The Orange curve represent this opportunity where starting temperature was 500 ($°C$) and at every calculation step it was decreased by 0,2 ($°C$). Recrystallization started but it wasn’t finished at the end of calculation. These results demonstrate that the developed automata can differentiate these recovery and recrystallization processes, and the coupling was successful.

4. Hot rolling simulation by 1D cellular automata

In the real factory practice approximately 400-500 (mm) thick semi continuous slabs are hot rolled to 5-8 (mm) final thickness in reverse rolling passes. Number of rolling passes could be different from 15 to 25. Between two hot rolling passes the material lays on roller table and it is cooling. The microstructure is changing during this time not just at hot deformation. Our automata were improved to simulate the material microstructure in case of hot rolling. This capability study focuses on one rolling pass and cooling period which is between two rolling passes. We can call the cooling period holding time. The first part of calculation is the rolling and second part of calculation is the cooling. At this stage the stored energy is an important factor therefore it was the main point in our experiment with recrystallized fraction. These were analyzed with modification of activations energies, recovery limit value and rolling speed. One additional calculation is necessary, the increment of the stored energy during the plastic deformation. For this the rolling operation is also divided by the same calculation steps, which is used by the simulation. Based on the geometry changes of the sheet - which recently calculated by geometric formulas by the rolling speed – the time scale becomes fixed, currently to 0.0001 (s/step). By the change of the thickness of the sheet an increment of the degree of deformation is calculated at every step. The 1D automata cannot hold a detailed information about the position and geometry of the represented material. But here in the simulation of hot deformation is a key question. In this study the universe
represents a small part of the cross section of the sheet. So, as the examined cross section passes through the rolls, with the introduced simple geometric model all cells make the same deformation. It can be refined with other detailed simulation of rolling process of course.

The mentioned increment of deformation per step means an increment of the stored energy. But this increment is depending on the current deformed state of the given cell, which is determined by the actual value of stored energy. To define the dependence between the stored energy and the degree of deformation the formula is used form \[ [10] \]

\[
E_{st}(\Delta h/H) = E_{stmax}(1 - \exp(-\Delta h/H))
\] (3)

\(E_{stmax}\) determine the shape of the curve, and 1 (kJ/cell) is used in current calculation. The algorithm of the calculation of stored energy increment is: 1. calculate the equivalent degree of deformation from the stored energy of the cell by (3); 2. increase the degree of deformation by the value of the actual calculation step; 3. calculate the new value of the stored energy by (3). This algorithm can be easily incorporated into the introduced automaton.

Figure 4-5. present the recrystallized fraction and stored energy in function of calculation steps where different nucleation activation energies (Qn) were used in calculations.

The other parameters were: \(Q_g=40\) (kJ/cell), \(Q_r=30\) (kJ/cell), \(E_{str}=800\) (J/cell), and the same values as presented above. The rolling speed was 1500mm/s. The hot rolling deformation phase was extended to 688 calculation steps and it is followed by a 2 (sec) cooling time which is present for 2000 calculation steps. Increased nucleation activation energy slows down recrystallization. Recrystallization starts at rolling and the smallest activation energy resulted in the highest recrystallized fraction. Recrystallized fraction is app. 5 (%) at the highest activation energy and app. 50 (%) at the smallest activation energy at 688 calculation steps in rolling zone. It can be seen also on figure 5, where curves have local maximum at this point. The maximum value is decreasing with decreasing activation energy that is coming from fast recrystallization and it is getting closer to the starting point of rolling. Recrystallization started sooner at smaller deformation and we got fully recrystallized structure in holding time.

5. Conclusion

The current study focused on the simulation of microstructural processes of hot rolling by 1D cellular automata. Hot rolling is a complex metal forming process where different physical processes are work hardening, softening (recovery and recrystallization). Cellular automata are a good method to simulate the microstructural changes and hence the changes in material properties. The big advantage of the 1D recrystallization automaton is that it calculates complex results next to its simplicity. This simulation was developed elsewhere and is applied for the study of recrystallization of OFHC copper where the recovery has no effect on the softening. In aluminum alloys during the annealing and hot rolling the recovery has a large effect on the mechanical parameters. A simple calculation is developed for recovery
and coupled with the 1D recrystallization automata. The most complex step of the aluminum sheet processing technology is the hot rolling. The developed automata are extended with a simple calculation of deformation and the changes of the stored energy and recrystallized volume fraction of the universe of the automaton are examined with different kinetic parameters as activation energies. The simple build-up of the introduced automata shows as complex behavior as the hot rolling step. This article introduced two extensions of the 1D automaton of recrystallization: the calculation of recovery kinetics and coupling it with the recrystallization simulation in that way that the new automata can simulate the kinetics of the mentioned processes during hot rolling and annealing too. This development makes possible to use the new automaton in the process simulation of production of rolled flat sheets. The automata can help a technology engineer to study the different changes of process parameters in the properties of the product. Currently the automata use arbitrary units in the calculation, so the scaling is important.

References
[1] Totten G.E. and MacKenzie D.S. at al 2003 CRC Press
[2] Hirsch J. Karhausen K.F and Engler O. et al 2004 Continuum Scale Simulation of Engineering Material
[3] Guo Z. and Saunders N. and Schillé J.P and Miodownik A.P et al 2009 Materials Science and Engineering vol 499 pp 7-13
[4] Marthinsen K. Holmedal B. Valle R. and Abtahi S. 2003 Materials Science Forum vol 426-432(5) pp 3777-3782
[5] Gottstein G, Crumbach M., Neumann L. and Kopp R. 2006 Materials Science Forum vol 519-521 pp 93-102
[6] Raabe D. et al1998 Computational materials science
[7] Bubonyi T. and Barkóczy P. 2018 IOP Conf. Ser.: Mater. Sci. Eng.426 012007
[8] Radhakrishnan B., Sarma G.B and Zacharia T. 1998 Acta materialia, Elsevier
[9] Midownik, M. A. et al 2002 Journal of Light Metals vol 2 pp 125-135
[10] Gyöngyösi Sz., Tóth A. and Barkóczy P. 2010 Materials Science Forum vol 659 pp 405-410
[11] Barkóczy P. and Gyöngyösi Sz. 2013 Materials Science Forum vol 729 pp 150-155
[12] Espericueta R. et al 1997 Cellular Automata Dynamics Math Department, Bakersfield College
[13] Farzadi A. et al 2015 Mat-wiss. u. Werstofftech vol 46, no. 12 pp 1218-1225