Development of a cellular automaton for a better consideration of elastic neighborhood effect in polycrystals

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Abstract

This paper presents the development of a cellular automaton (CA) which could take into account the neighborhood effect in the context of polycrystal mechanics. This model aims to have a better estimate of the stress / strain field in polycrystals than conventional analytical models such as the self-consistent model (SCM). As the first step in the consideration of neighborhood effect, the model was developed in the case of a uniaxial loading in linear elasticity. A Kelvin structure is used to represent a polycrystal, considering that all grains have the same size and shape. The primary focus is the influence of crystallographic orientations on the local behavior in the microstructure. The model has been developed based on the hypothesis that the Finite Element Method (FEM) can quantify correctly the influence of a grain's neighborhood on its behavior. FEM, SCM, and the analytical model results are finally compared grain by grain after simulations on 686 grains polycrystalline aggregates in the Kelvin structure. The results show that the developed CA provides an approximation almost three times better than those of the SCM and the importance of taking into account the neighborhood effect. This also gives an opportunity to better understand the parameters that influence the behavior of a grain in a polycristal.

Keywords: Cellular automaton, Homogenization Model, Anisotropy, Eshelby's inclusion, Polycrystal, Neighborhood.

Introduction

The Finite Element Method (FEM) is the most common method used to simulate the micromechanical behavior of polycrystals [1, 2]. It requires a heavy amount of computer resources and the analytic model such as the Self-Consistent Model (SCM) [3] can offer a good approximation of the micromechanical behavior of polycrystals for a much lower calculation time, allowing for the possibility to simulate various microstructure configurations. However, the SCM does not take into account the neighborhood effect as each phase is defined solely by its crystal orientation and volume fraction, and there is no spatial representation of the polycrystal.

This is quite unfortunate as the neighborhood effect is an important criterion to consider if one wants to describe the behavior of the material on a local scale [4]: a grain surrounded by soft grains will not show the same behavior as the same grain surrounded by hard grains. In order to take this into account, the principles of the cellular automaton model have been considered by several authors to address this limitation [5, 6, 7]

A cellular automaton (CA) is a discrete mathematical model where the structure is discretized into several cells. Each cell has a characteristic initial state that characterizes it, and its behavior

Table 1: Elastic constants of the cubic iron crystal ([11])

Fe	$C_{1111} = 226$ GPa	$C_{1122} = 140$ GPa	$C_{1212} = 116$ GPa

depends on the behavior of its neighboring cells. This is described by a transition rule. Such CA can describe and predict complex behaviors in many different fields of research [8, 9, 10].

In this context, the objective of this research is to develop a simple model based on the SCM by adding the principles of CA in order to take into account the neighborhood effect. As a first step, the structure of Kelvin (Fig.1) has been used to annihilate the effects of grain shape and size ratio, and to document only the effect of grain orientation of the neighboring grains. Non cristallographic texture was introduced in the microstructure. They were tested in uniaxial loading with linear elasticity properties. In order to have a better understanding of the influence of the neighborhood of a grain, a full-field numerical study has been proceeded using the FEM. From the hypotheses that FEM simulation gives "the right" results, a model has been developed and its results have been compared with the ones obtained by FEM approach.

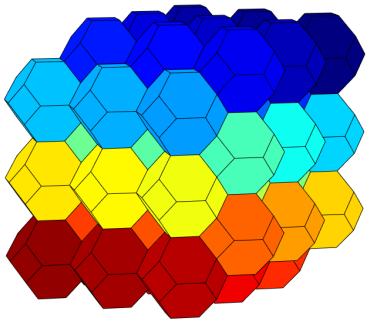

Figure 1: Kevin Structure

The material properties used in the results shown in this paper are the properties of the iron crystal (Tab.1)(Cubic elastic tensor), but the approach was also applied to other materials such as Aluminium, Nickel or Titanium with similar accuracy.

Comparison of the FEM and the SCM

FEM simulations have been performed on a cube of 686 grain, with 20 different crystallographic orientation distributions on a Kelvin structure (Fig. 1) to simplify the study of the neighborhood effect and cancel any size and shape effect (all grains are identical). Periodic boundary conditions have been applied in order to cancel any border effects. Arbitrarily, a uniaxial loading $\underline{\underline{E}}^0$ is applied to the cube, where $E_{ij} = 0$ except for $E_{33} = 0.1\%$. The resulting effective stress is $\Sigma_{1st}^{eff} = 274$MPa. The crystals are purely elastic, and the elastic tensor of the iron crystal (Tab.1) has been used for all the simulations that are presented in the rest of the paper.

On Fig.2 are presented the mean first principal stress in each grain obtained with the FEM and the SCM. For a given grain Young modulus, the FEM shows a dispersion of the stress where as the SCM shows only one possible stress solution to the problem. The SCM is actually an average of the stress observed with the FEM. This dispersion is clearly related to some neighborhood effect. With some neighborhood conditions, that could lead to significant increase of the local stress compared to the SCM. The highest stress observed with the SCM is approximately 108% of Σ_{1st}^{eff} when the highest stress observed with the FEM is 120% of Σ_{1st}^{eff}.

Study of the neighborhood effect

The SCM showed to have a good first approximation of the stress in the grain but it clearly needs to be corrected to consider the neighborhood effect and predict more realistic and statistical results. In order to do that, the influence of one or several grains on a given grain has been studied depending on their spacial and crystal orientation distribution.

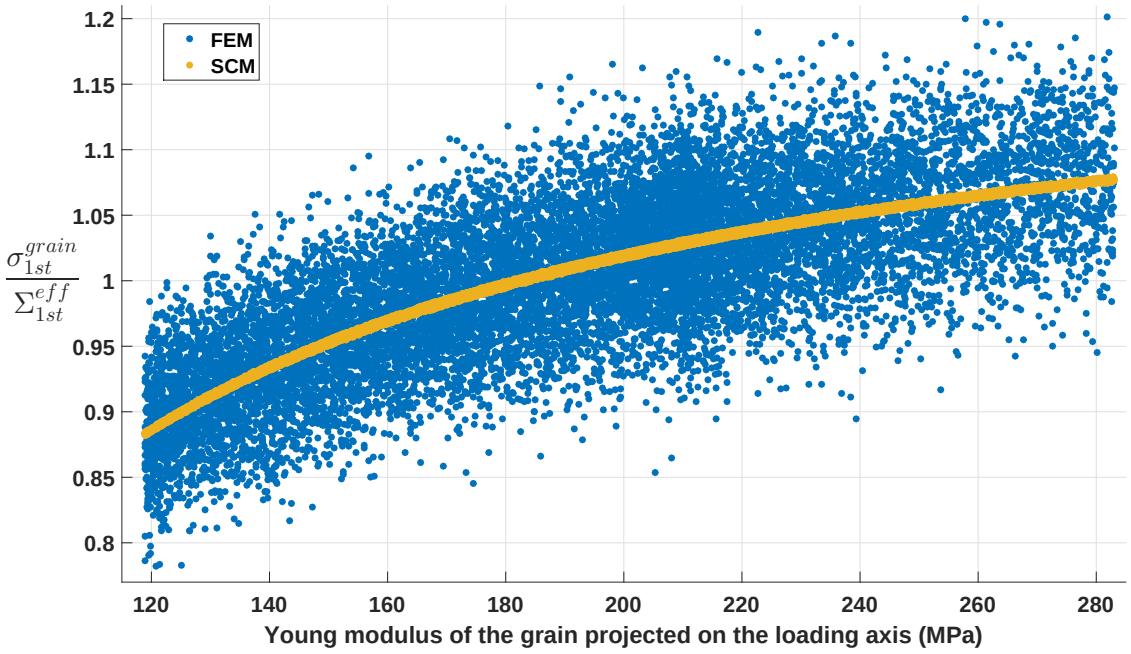

Figure 2: First principal stress in each grain of the polycrystal normalized by the macroscopic first principal stress: Comparison between the FEM and the SCM

Grain interaction

In order to see the influence of one grain on an other grain in the polycrystalline Kelvin structure, the behavior of two grains A and B immersed in an infinite homogeneous matrix has been documented as a function of their crystal orientations and their relative position.

Firstly, the macroscopic properties of the material are attributed to the homogeneous matrix and the central grain A, and crystallographic properties are attributed to grain B.

The first principal stress of grain A (0;0;0) has been observed depending on the position X, Y, Z and the crystal orientation of grain B. An influence factor α_B^A of grain B on grain A is defined such as $\alpha_B^A = \sigma_B^A/\sigma_0^A$, where σ_0^A is the first principal stress of grain A immersed alone in the matrix and σ_B^A is the first principal stress of grain A immersed in the matrix with grain B.

It was found that if the elastic tensor $\mathbb{C}_B$ of grain B is expressed in the local base where the axis Z is parallel to the loading axis and the axis X points toward the projection of grain B on the plan perpendicular to the loading direction (Fig. 3), the components $\mathbb{C}_{3333}$, $\mathbb{C}_{1133}$ or $\mathbb{C}_{3313}$ of this elastic tensor $\mathbb{C}_B$ directly influence the factor α_B^A (Eq.1).

$$\begin{aligned}\alpha_B^A(X,Y,Z) = a_1^{(X,Y,Z)} &\times \mathbb{C}_{3333} \\ + a_2^{(X,Y,Z)} &\times \mathbb{C}_{1133} \\ + a_3^{(X,Y,Z)} &\times \mathbb{C}_{3313} \\ + a_4^{(X,Y,Z)}&\end{aligned} \quad (1)$$

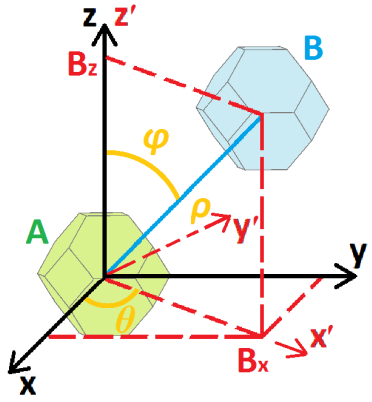

Figure 3: Illustration of the local base formed by grains A and B

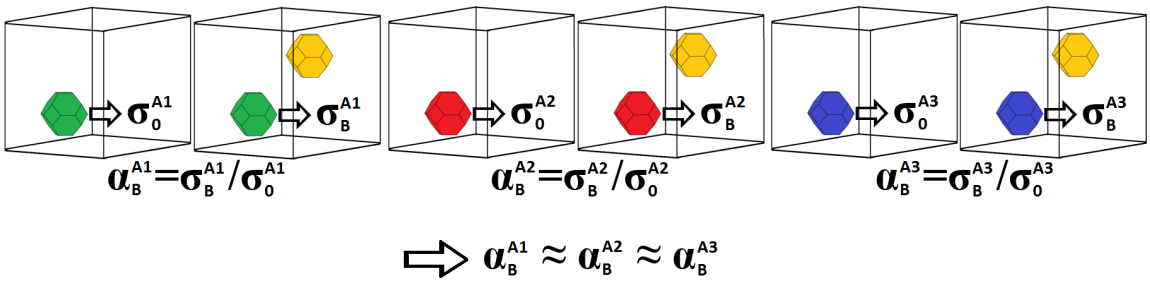

Figure 4: Illustration of the first assumption (each color corresponds to a different crystallographic orientation): the influence of grain B on grain A is independent of the orientation of grain A

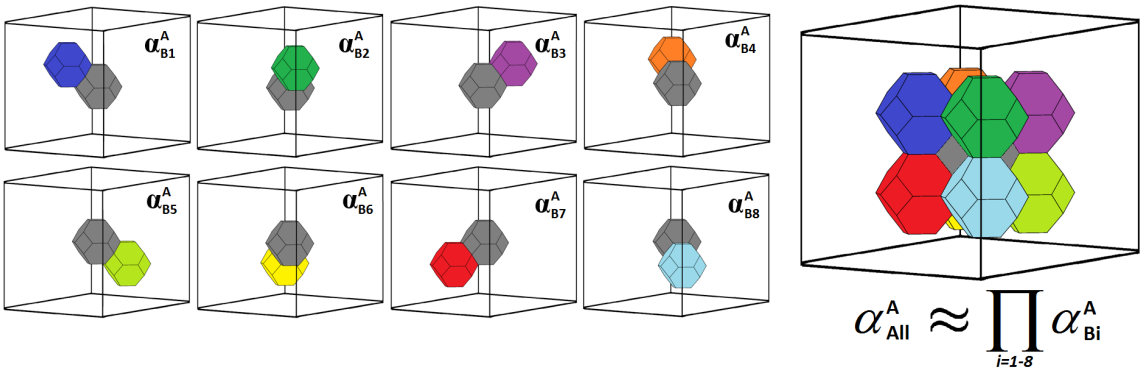

Figure 5: Illustration of the influence of each individual grain compared to the influence of several grains (each color corresponds to a different crystallographic orientation): the influence of several grains is equal to the product of the influence factor of each neighboring grain

The coefficients $a_i^{(X,Y,Z)}$ are calculated from the FEM results for each different relative position (X;Y;Z).

The calculations were run with grain A having the effective properties of the material. In order to generate the equation for any orientation of grain A, the crystal properties are attributed to grain A and calculations are run. It has been observed that the influence of the crystal orientation of grain A is negligible compared to the influence of the crystal orientation of grain B, suggesting a first assumption for the model under development: the influence of grain B on grain A is independent of the orientation of grain A (Fig.4). With that assumption made, equation 1 can be used to calculate the influence factor α_B^A of grain B on grain A for any crystal orientation of grain A.

Influence of several grains on another grain

The influence of several grains on the central grain A has been studied. Knowing the influence factor α_{Bi}^A of each neighboring grain Bi on grain A, it has been observed that the influence of several grains on grain A is equivalent to the product of the influence factor of each neighboring grain (Fig.5). A second assumption can be made: the influence of several grains is equal to the product of the influence factor of each neighboring grain (Eq.2)

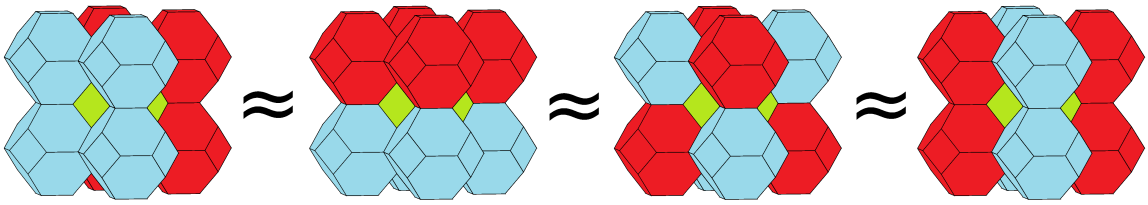

Figure 6: Illustration of the influence of several grains with the same set of influence factors but with different repartitions (the grains in blue correspond to the lowest influence factor α^A_{Bmin} and the grains in red to the highest influence factor α^A_{Bmax}): the influence of a neighboring grain on the central grain is not affected by the other neighboring grains.

$$\alpha^A_{All} = \prod_n^N \alpha^A_n(x, y, z, \varphi_1, \Phi, \varphi_2) \tag{2}$$

A consequence of the latter observation and assumption is that the distribution of the neighborhood doesn't affect the results as long as the α^A_{Bi} values do not change. In figure 6 are illustrated 4 neighboring grains with the lowest influence factor α^A_{Bmin} and 4 other neighboring grains with the highest influence factor α^A_{Bmax} distributed differently. It is observed that no matter how those grains are distributed, the stress in the central grain is not significantly affected (Fig.6). A third assumption is made : the influence of a neighboring grain on the central grain is not affected by the other neighboring grains.

Definition of the Cellular-Automaton

Based on the three assumptions declared in the previous chapter, a cellular-automaton (CA) has been developed using Self Consistent calculations to evaluate the first principal stress σ^A_0 of grain A. The solution σ^A_{SCM} of the SCM for a spherical inclusion with the elastic property of grain A (a Kelvin structure's cell can be considered as spherical) immersed alone in the matrix was used as the base for the calculation. The CA solution consists of applying to the SCM solution the influence factor of each neighboring grain that is considered to have a significant influence:

$$\sigma^A_{AC} = \sigma^A_{SCM} \times \prod_n^N \alpha^A_n(\underline{X}, [\varphi_1; \Phi; \varphi_2]) \tag{3}$$

In Eq.3, N is the number of neighboring grains considered, $\underline{X}$ is the vector form by grain A and the neighboring grain n, $[\varphi_1; \Phi; \varphi_2]$ are the Euler angles representing the orientation of the neighboring grain n, and the influence factor α^A_n of grain n on grain A is calculated with the Eq.1.

Results of CA calculation are shown in Fig.7 and 8, presenting the first principal stress in each grain obtained with the FEM and the CA. Four types of neighborhood are presented:

- 0 neighboring grain is considered. In other words, this is the SCM results.
- The first layer of neighboring grains are considered ($N = 14$ grains): all neighboring grains that have a distance from the central grain $d \leq 2r$, where r is the radius of one grain.
- The second layer of neighboring grains are considered ($N = 64$ grains): $d \leq 4r$.
- The third layer of neighboring grains are considered ($N = 258$ grains): $d \leq 6r$.

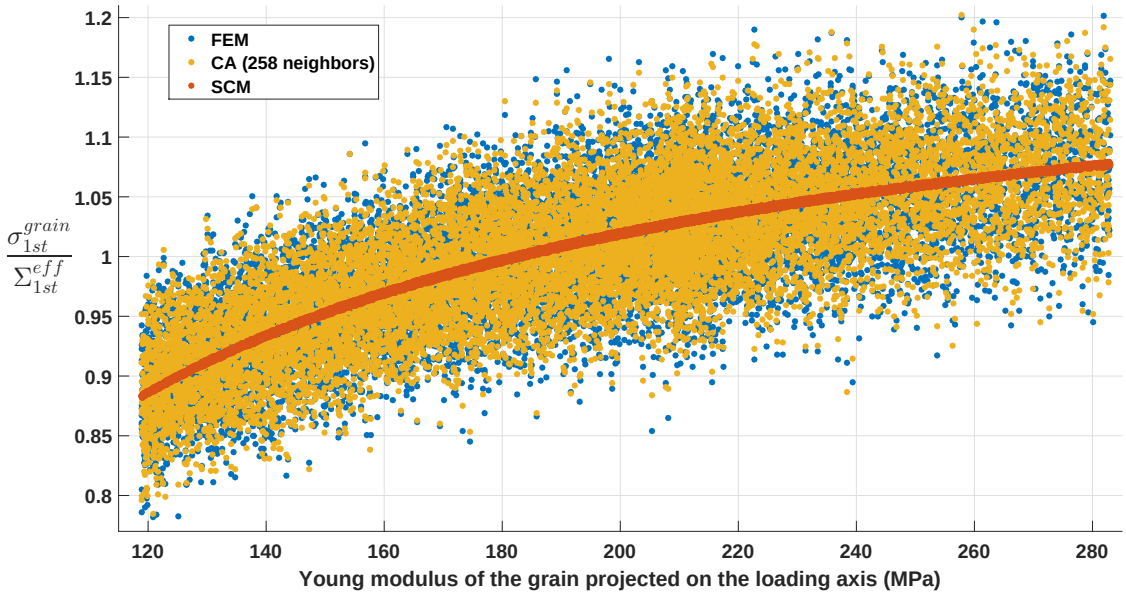

Figure 7: First principal stress in each grain of the polycrystal normalized by the macroscopic first principal stress: Comparison between the FEM, SCM, and CA

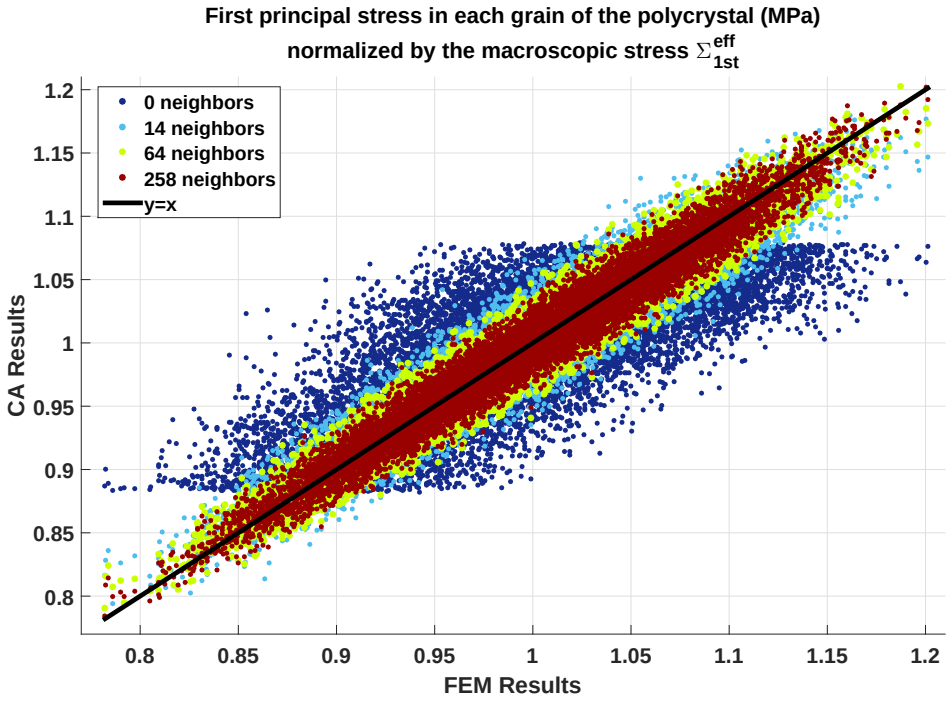

Figure 8: Comparison of the FEM results with the CA results

Table 2: Comparison of the FEM results with the CA results

	$N = 0$	$N = 14$	$N = 64$	$N = 258$
Normalized average difference $\left\langle \frac{\left\lvert \sigma_{EF}^{grain} - \sigma_{SC}^{grain} \right\rvert}{\Sigma_{EF}^{eff}} \right\rangle_{grain}$	3.42%	1.59%	1.22%	1.04%
Normalized maximum difference $max_{grain} \left(\frac{\left\lvert \sigma_{EF}^{grain} - \sigma_{SC}^{grain} \right\rvert}{\Sigma_{EF}^{eff}} \right)$	16.93%	8.80%	5.78%	5.41%

In Fig.7 are presented the FEM, SCM and CA (with 258 neighboring grains considered) results. As we can see, consideration of the neighborhood effect in the model generates a dispersion of the stress similar to the one observed for the FEM results. If we take a closer look at the local behavior on Fig.8 and Tab.2, it is observed that the more neighboring grains are considered, the closer the CA results are to the FEM ones. The accuracy of the CA with $N = 258$ is three times better than a simple SCM, and the extreme values are better captured. For information, using the same computer, the FEM simulation takes approximately 40 minutes to be completed when the CA with $N = 258$ takes 40 seconds.

Conclusions

The present work shows the importance of the neighborhood effect in polycrystal fields. From the observations of the Finite Element simulations, a cellular automaton has been developed taking into account the neighborhood effect. The model is based on the Self-Consistent model to which an influence factor is applied depending on the orientation and distribution of the neighborhood of the grain. Taking the FEM results as a reference, the model showed a significant improvement of the results compared to the original SCM.

References

[1] Forest, S., Cailletaud, G., Jeulin, D., Feyel, F., Galliet, I., Mounoury, V. and Quilici, S. (2002) Introduction au calcul de microstructures. Mecanique et Industries **3**, 439-456.

[2] Roters, F., Eisenlohr, P., Hantcherli, L., Tjahjanto, D. D., Bieler, T. R., Raabe, D. (2010) Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications. Acta Materialia **58**, 1152-1211.

[3] Kroner, E. (1961) Zur plastischen verformung des vielkristalls. Acta Metallurgic **9**, 155-161.

[4] Kocks, U. F., Tom, C. N. and Wenk, H. R. (1961) Texture and Anisotropy. Preferred Orientations in Polycrystals and Their Effect on Material Properties. Cambridge University Press.

[5] Montheillet, F. and Gilormini, P. (1996) Predicting the mechanical behavior of two-phase materials with cellular automata. International Journal of Plasticity **12**(4), 561-574.

[6] Boutana, N. and Bocher, P. and Jahazi, M. (2008) Discrepancy between fatigue and dwell-fatigue behavior of near alpha titanium alloys simulated by cellular automata. International Journal of Fatigue **51**, 49-56.

[7] Pourian, Meysam H. and Pilvin, Philippe and Bridier, Florent and Bocher, Philippe (2014) Heterogeneous elastic behavior of HCP titanium polycrystalline aggregates simulated by cellular automaton and finite element. Computational Materials Science **92**, 468-475.

[8] Hesselbarth, H.W. and Gbel I.R. (1991) Simulation of recrystallization by cellular automata. Acta Metallurgica et Materialia **39**(9), 2135-2143.

[9] Ding, R., Guo, Z.X. (2002) Microstructural modelling of dynamic recrystallisation using an ex-

tended cellular automaton approach. Computational Materials Science **23**, 209-218.
[10] Solas, D., Thbault, J., Rey, C., Baudin, T. (2010) Dynamic Recrystallization Modeling during Hot Forging of a Nickel Based Superalloy. Materials Science Forum **638**, 2321-2326.
[11] Simmons, G. and Wang, H.F. (1971) Single crystal elastic constants and calculated aggregate properties: a handbook. The M.I.T. Press **2**.