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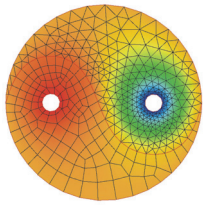

SOME ASPECTS WHICH DENY A USE OF 2D CELLULAR AUTOMATA FOR MODELING OF RECRYSTALLIZATION

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Abstract

The main reason why the two-dimensional cellular automata (2D CA) are preferred to the three-dimensional (3D) ones is time of calculations. A number of cells in the 2D CA is the second power of space size, while in the 3D CA it is the third power. It pertains to a number of neighboring cells as well. Then the cost of the 3D calculation is higher than that of the 2D calculation more than the space size of the CA. It means that simulation in the 3D CA of the linear size of 100 cells demands more calculations than 100 simulations in the 2D CA of the same size. The CA is used for modeling of crystallization, recrystallization, phase transformation, crack propagation, micro-shear band and shear band propagation. But can the 2D CA hold up a mirror to the real process? In the paper some aspects of the using of the 2D CA for the recrystallization are considered. Four main problems, which can be solved or at least can be accounted, are dealt with here. Those are kinetics of the recrystallization, a nucleation, a grain growth rate and deformation of grains. Some of the problem can be solved for the static recrystallization but not for the dynamic one. Some proposals and recommendation are included in the paper.

Key words: microstructure, modeling, cellular automata, recrystallization

1. INTRODUCTION

Recently an interest to applying of the cellular automata (CA) for the simulation of different phenomena in materials is arisen constantly. The cellular automation is used for modeling of crystallization (Rappaz & Gandin, 1993; Raabe, 2004; Burbelko, 2004), dynamic and static recrystallization (Davies, 1997; Hurley & Humphreys, 2003; Qian & Guo, 2004), phase transformation (Kumar at al., 1998), cracks propagation (Das at al., 2002), micro-shear band and shear band propagation (Makarov & Romanova, 2000) etc. The main asset of the CA is ability for a close correlation of the microstructure with the mechanical properties in micro- and meso-scale simulation. It allows for visualization of results microstructure simulation as well. The finite element method is the most accurate and the most frequently used for thermo-mechanical modeling in macro-scale. The CA method is only intended to play the same role in micro- and meso-scale. Joining both of them undoubtedly improve accuracy of modeling of coupled phenomena during the forming processes in both micro- and macro-scale. Models for simulation of the recrystallization based on the CA are developed and recently used prevailing in two-dimensional (2D) version (Kugler & Tukr, 2006; He at al., 2006, Kroc 2005, Raabe & Hantcherli, 2005). Though, three-dimensional (3D) models are also available (Ding at al., 2006). The 2D CA have some advantage over the 3D CA. Models based on the 2D CA are the simpler and faster, have less elements and connections, use less complicated algorithms, are simpler for design, implementation, more useful

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for visualization. Some problems, such as accounting of a crystallographic orientation of the grains or curvature of grains boundaries, which have been solved in the 2D CA, are still unsolved in the 3D CA. Microstructure evolution is pointedly theedimensional and results obtained by the 2D CA not always can be transferred to a real 3D process directly. Four main problems, which can be solved or at least can be accounted in 2D CA, are presented below. Those are kinetics of recrystallization, a nucleation, a grain growth rate and deformation of grains.

2. KINETICS OF RECRYSTALLIZATION

Avrami (1939) for the recrystallization kinetics calculations has proposed to use the extended volume V_{ex} that is the total transformed volume if overlapping of the growing grains is neglected. Then the recrystallization fraction χ can be calculated via extended volume as following:

$$\chi = 1 - \exp(-V_{ex}), \tag{1}$$

where V_{ex} can be expressed as following: $V_{ex} = \beta t^n$, β and n are coefficients, which depend on nucleation $\dot{N}$ and grain growth rate $\dot{D}$.

If we consider a recrystallization process with a constant nucleation rate $\dot{N} = const$ and isotropic grain growth rate $\dot{D} = const$, the coefficient n is equal to 4. In a case of nucleation before the grain growth $\dot{N} = 0$ and $n = 3$. The coefficient n is completely defined by the cubic dependence grain volume V on its size D: $V = N\frac{\pi D^3}{6} = N\frac{\pi \dot{D}^3}{6}t^3$.

In the 2D CA, it is impossible to receive the same cubic dependence, it will be square-law only: $V_{2D} \equiv S = N\frac{\pi \dot{D}^2}{4}t^2$. In the recrystallization process with anisotropic growth (preferential growth in the two directions) the 2D CA can be used if the axes, which the grain growth rate is close to zero in, of all grains are coincided. Then results will be proper not only for the recrystallization fraction but also for the form of crystallites in the cross-section correspondent to the two directions of the preferential growth. If the axes are not coincided, the grain growth rate must be differentiated for each grain. The flat grains in the cross-section degrade to the line and the coefficient n for those grains is reduced to 1. Therefore the result is wrong.

There can be received $n = 3$ in the 2D CA when the nucleation lasts during the whole recrystallization process. Accordingly, the 2D CA with the nucleation during the recrystallization can simulate a process with the nucleation before the grain growth. Then the 2D CA can simulate static recrystallization, which is corresponded to abovementioned nucleation condition. Validity of that approach can be shown below. It respects anisotropic growth as well.

On the other hand the approach cannot be used for the dynamic recrystallization process, where new nuclei appear all the time. Here one can approximate the quartic dependence by the cubic one. It is impossible to do exactly. In figure 1 are shown some curves calculated according to equation (1) for three values of coefficient n. If n is set, one can change the coefficient β (1) only. The curves in figures 1a and 1b are differed by coefficients β. If one parameter can be used for approximation, the only one point on the curves is coincident. In figure 1a, the time of the recrystallization for three variants are the same ($t_{0.95} = 5$ s), in figure 1b, the time, when fraction equal to 0.5, is the same ($t_{0.5} = 3$ s). In both variant full coincidences is impossible. Almost ideal fitting can be obtained when delay τ for an initiation of the recrystallization process is introduced ($t \rightarrow t - \tau$), as it is shown in figure 1c. That approach commonly used not only in CA. So, the delay for dynamic recrystallization is introduced indirectly by the addition of the critical strain ε_{cr}, stress σ_{cr} or dislocation density ρ_{cr} for the initiation of the recrystallization process. Then the main difference between two processes described by different coefficient n is in the additional delay for smaller n. For $n = 4$ the delay is absent, for $n = 3$ it must be introduced and its dependence on the parameters of the deformation must be established additionally.

The nucleation $\dot{N}$ and the grain growth rate $\dot{D}$ cannot be defined properly either. To receive the proper average grain size after the recrystallization it is enough to have a proper number of grains N because $D^3 \propto 1/N$ or $D^2 \propto 1/N$. If curves are fitted (as in figure1c) the times of the recrystallization are differed in time of delay. Then the same grain size is received in shorter time ($\dot{D}_{2D} > \dot{D}_{3D}$). The nucleation lasts shorter as well ($\dot{N}_{2D} > \dot{N}_{3D}$). The less is the fraction of the recrystallization the bigger error in number of grains and its size. During the process following dependences can be written:

$D_{2D} = \frac{(t-\tau)t_{0.95}}{(t_{0.95}-\tau)t} D_{3D}$ $N_{2D} = \frac{(t-\tau)t_{0.95}}{(t_{0.95}-\tau)t} N_{3D}$, ie. $D_{3D}>D_{2D}$, $N_{3D}>N_{2D}$. It almost has not influence on the curve, but when the dynamic recrystallization does not complete, the further post-dynamic recrystallization would go different way.

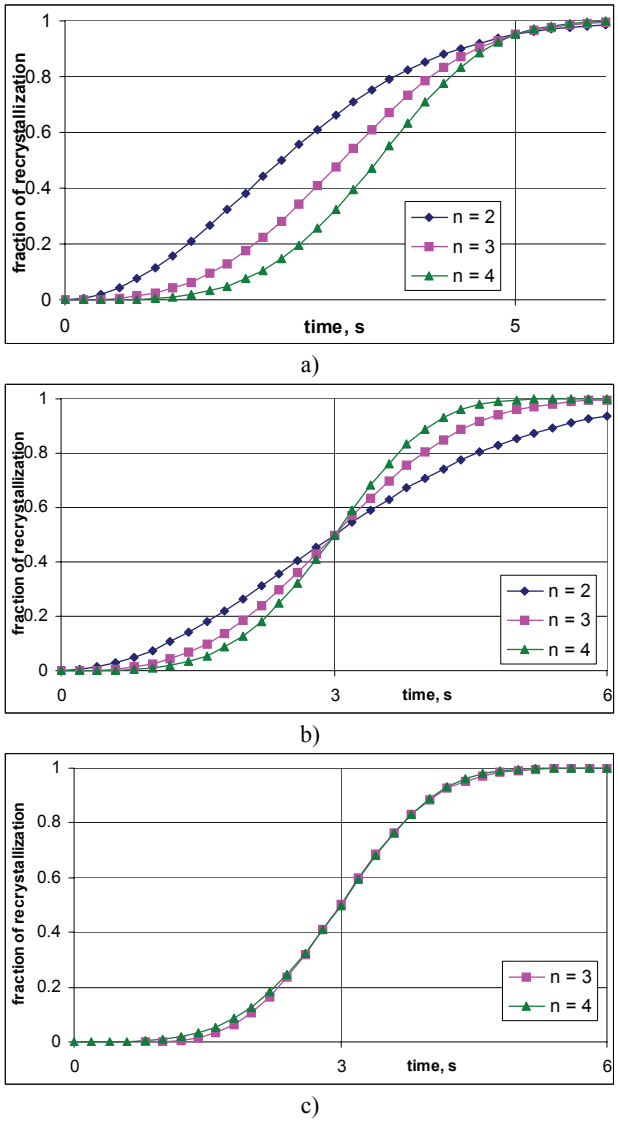

Fig. 1. *Fraction of the recrystallization calculated according to equation (1): a) $t_{0.95}$ = 5 s, b) $t_{0.5}$ = 3 s, τ = 0 s, c) $t_{0.5}$ = 3 s, for n = 3 τ = 0.8 s.*

The size of the grains during the dynamic recrystallization must be unreal as well. Obtaining of the same fraction of the dynamic recrystallization is supposed an appearing of new volume free of dislocations. Then to receive the same values of the fraction χ for 3D and 2D one can write the following: $\chi = \frac{\Delta V_{3D}}{V_{3D}} = \frac{\Delta S_{2D}}{S_{2D}}$. The new volume ΔV_{3D} (ΔS_{2D}) can be expressed in terms of the boundary surface S_{3D} (L_{2D}) of growing grains and the grain growth rate $\dot{D}$. Then $\frac{S_{3D}\dot{D}_{3D}\Delta t}{V_{3D}} = \frac{L_{2D}\dot{D}_{2D}\Delta t}{S_{2D}}$ and if equal grain growth rate is supposed ($\dot{D}_{3D} = \dot{D}_{2D}$), $\frac{S_{3D}}{V_{3D}} = \frac{L_{2D}}{S_{2D}}$. Finally by expressing those ratios via the grain size D_{3D} (D_{2D}) one receives a following dependence: $D_{3D} \cong 1.5 D_{2D}$. In other words for the equal grain growth rate $\dot{D}$ in the 2D CA the average grain size must by less than that in the 3D CA ($D_{2D}<D_{3D}$) or in the real process. And on the contrary, if $D_{3D}=D_{2D}$ is supposed, $\dot{D}_{2D} \cong 1.5\dot{D}_{3D}$. It has respect to the full dynamic recrystallization as well.

Thus, when equalities of the grain sizes $D_{3D} = D_{2D}$, the nucleation rate $\dot{N}_{2D} = \dot{N}_{3D}$ and the grain growth rate $\dot{D}_{2D} = \dot{D}_{3D}$ are supposed, a direct contradiction with the assumption is received, namely: $D_{3D} > D_{2D}$. A conclusion is obvious: the 2D CA allows one to receive either kinetics of recrystallization or proper microstructure (the average grain size and maybe grain size distribution) but not all of them.

3. NUCLEATION

It is well known that the preferred location for the nucleation is on the boundaries of the grains. It is the main assumption of most CA as well. The 2D CA is considered as a cross-section. But is the assumption true for the case? Why does one believe that the nuclei appear on that cross-section only? And why cannot grains appeared outside grow into the cross-section? Obviously, for the cross-section it is seemed as the nucleation occurs not only on the boundary of the grains. The second consequence is that there is the appropriate time (delay) required for the nuclei appeared outside to have growed up to the cross-section.

Then in order to model the static recrystallization by the 2D CA, when the nuclei appear before the process begins, the continuous nucleation during the whole process of the grains growth must be assumed. If at the beginning the nuclei appear on the boundary, by the end their appearance displaces to the center of the grains. The grain growth rate and rate of nucleation displacement must be coordinated. There can be established a ratio of these two rates. The ratio must account a shape of the grains, mainly a size in the third direction (perpendicular to cross-

section). This problem can be easily solved and used in the modeling. Here is enough to add to the description of the grain parameters (or better to each cell of the CA) two values for the grain boundary: above and below the cross-section. Moreover the values must not be discrete. Then the locations of the nucleation are determined. After that the new grains grow into the cross-section and in the separated sells. When the growing grain in the cell reaches the cross-section, it corresponds to the nucleation in the cell. And finally the grain is growing in the cross-section. In fact that is 3D calculations on the base of the 2D CA. In that way a layer of grain is considered here instead of the cross-section.

The problem is complicated when one tries to model the dynamic recrystallization. The continuous nucleation during the recrystallization must be reckoned. The nuclei appear on secondary boundaries as well. But a location of the boundaries is unknown. Then the nuclei must be thrown in the space of the CA randomly. It maybe allows for receiving proper kinetics of the recrystallization, but there remains the problem of the grain size described above and a problem of the grain growth rate, which is presented below.

4. GRAIN GROWTH RATE

In the 3D CA every rule for the grain growth rate can be used on the strength of the theory requirements whereas in the 2D CA an implementation of even a constant linear velocity for the boundary movement demands a great care. In the simplest variant, when the new grains appear on the cross-section, task do not differ from a variant of the 3D CA. Velocity in all directions is equal to a predetermined value. The nucleation outside the cross-section makes the matters worse. Further explanations are based on figure 2.

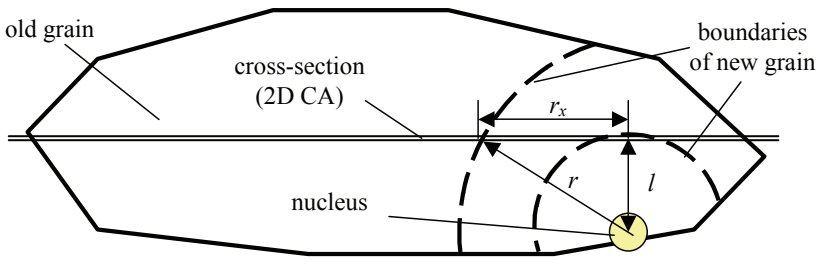

Fig. 2. *Scheme for the calculation of apparent velocity of the boundary movement.*

Let a nucleus appears on the boundary of old grain. A new grain grows from the nucleus with the constant linear velocity v (or half of the grain growth rate $v = \dot{D}/2$). On the front-view a boundary of the grain seems as a part of circle. The nucleus lies on the distance l from horizontal cross-section (that is the 2D CA). So, the nucleation is transpired on the layer of the 2D CA with a delay $\tau = l / v$. After that grain is growing on the 2D CA, but an apparent velocity v_x in the horizontal cross-section is not equal to the real velocity v. A real radius of the grain is $r = vt$, while an apparent radius in the 2D CA is r_x, which can be calculated as following: $r_x = \sqrt{v^2t^2 - l^2}$. Then the apparent velocity is $v_x = \frac{dr_x}{dt} = \frac{v^2 t}{\sqrt{v^2t^2 - l^2}}$. An example of the changes of the apparent velocity v_x is presented in figure 3. At the first moment, when boundary of the new grain reaches the layer of the CA, the apparent velocity is infinite. Then it drops and finally asymptotically reaches to the predetermined value.

For the static recrystallization it can be taken into account, meanwhile for the dynamic recrystallization it appears to be very difficult. There must be determined the distance from the layer of the CA, but for the DRX it remains indefinite.

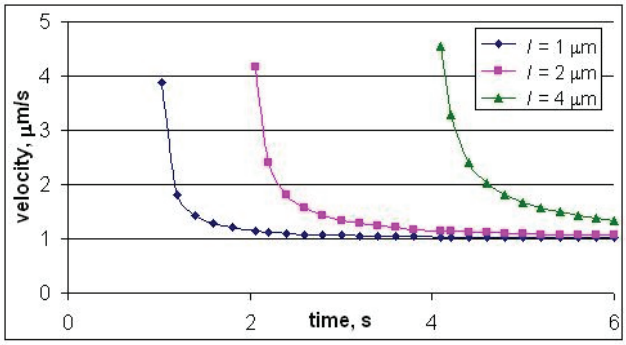

Fig. 3. *Apparent velocity of the boundary movement in the cross-section (a layer of the 2D CA).*

In the case of the static recrystallization, when the nuclei are appeared in the same moment and the grain growth rate is the same for every new grain (or change according to the same law), the grains boundary have to be flat, perpendicular to the line connected locations of nuclei appearance. That can evidence for proper simulation of static recrystallization (figure 4a). In the 2D CA without consideration of the algorithm described above, one receives either improper kinetic of recrystallization or curve boundaries. If grain growth

rate is the same, but appearance time is different, shape of boundary will be a hyperboloid in the 3D or a hyperbola in the 2D case (figure 4b).

5. DEFORMATION OF GRAINS

Unfortunately in the science literature Author fails to find accounting of the grain deformation when dynamic recrystallization is modeled by the CA. Obviously it lowers value of results of those researches. The problem has not resolve yet, some propositions are presented by Svyetlichnyy (2006). Nonetheless correct accounting of the grain deformation in the 2D CA is possible for the plane strain only. In the other case, area of the gross-section of the grains as well as the sizes of the elementary cell of the CA must be changed, that introduces an additional error.

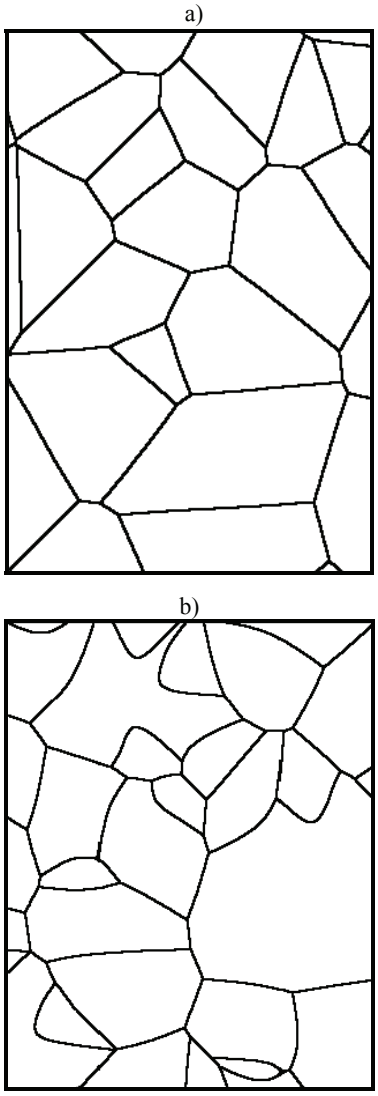

Fig. 4. *Shapes of the boundaries: a) flat boundaries when the nuclei appear before the grain growth, b) hyperbolical boundaries when the nucleation last during the grain growth.*

Here must be a remark about the boundary condition of the space. For the modeling of the microstructure and the recrystallization is mainly used a periodic boundary condition, when the top of the space is connected with the bottom as well as the left side is connected with the right side. The connections establish space as a torus. The periodic boundary conditions are used both in the 2D and the 3D CA because it allows for receiving the same results in somewhat smaller space. When the open boundaries are used, the space near the boundaries gives some error that can be accounted. The periodic boundary conditions can be remained during the deformation provided axes of the CA are coincident with the principal strains; otherwise open boundaries must be used. Moreover the deformation must be homogeneous in the whole space. The coincidence with the principal strains means the shear deformations do not appear. Shear strain causes an appearance of the discontinuous on the cohered boundaries and as result one, two or all three boundaries connections must be broken. In the case of the open boundary conditions, the deformation can be heterogeneous and final shape of the space can be arbitrary, for example, coincident with the deformed element used in FEM simulation.

6. WHY IS THE 2D CA PREFERRED TO THE 3D CA OR THE 1D CA?

The main reason why the 2D CA is preferred to the 3D CA is time of calculations. The number of cells in the 2D CA is the second power of space size, while in the 3D CA it is the third power. It pertains to the neighborhood of the cells as well. Then the cost of the 3D calculations is higher than that of the 2D calculations more than the first power of the space size of the CA. It means that modeling in the 3D CA of the size of 100 cells by the simple direct algorithms demands more calculations than the 100 modeling in the 2D CA of the same size. An analogous relationship exists between the 2D and the 1D CA. Then the following question arises. Why does nobody prefer the 1D CA to the 2D CA? Intuitively everybody feels that the 1D CA is worse than the 2D CA, and if the 2D CA is not the best variant, the 1D CA will be the worst one. Is it always true? Let's consider some disadvantage of the 1D and the 2D CA in the order as above.

The kinetics of recrystallization. The time dependence in the equation (1) for the 1D, 2D and 3D CA for static recrystallization is of the first, second

and third order respectively or for dynamic recrystallization is of second, third and forth order. If the 2D is considered as a cross-section, then 1D will be a line drawn on the cross-section. It is not obligate that the cross-section is of maximal area as well as size in the 1D CA is equal to the grain size. But in consideration of some assumption one can recalculate grains volume from the area of cross-section as well as from the average size of grains in the 1D CA. The latter recalculations are simpler. Moreover the one of the practical method of grain size calculation is based on the calculation of the number of boundaries (grains) on the line drawn on the cross-section. It responds to the 1D CA. For the higher accuracy one can use several 1D CA, all the same, time of calculations will be shorter than that for the 2D CA.

Nucleation. For both the 2D and the 1D CA nuclei must appear everywhere, not only in the boundary. Then there is no difference between those two approaches. For the 1D CA one can use the same algorithm, which is described above, with a small modification. For the some cell will be set a distance to the nucleus. While for the 2D CA it was a line perpendicular to the cross-section, for the 1D CA it is a plane perpendicular to the line.

Grain growth rate. A reasoning for the grain growth rate in the 1D CA does not differ from the one for 2D CA at all. Time dependence of the grain growth rate is the same, only distance is calculated in two coordinates instead of three coordinates for the 2D CA.

Deformation. That problem can be easily solved neither for the 2D nor the 1D CA.

As resume from the comparison of 1D and 2D CA can be following. Results obtained by the 1D CA not always, not obligatory are worse than that obtained by the 2D CA. But the calculation time is severely shorter.

The other question is when the 1D, the 2D or the 3D CA has to be used. An answer depends on the problem to be solved. If one interests in the kinetics of the static recrystallization, there does not need any CA, neither 3D, nor 2D, nor 1D. Here is enough the equation (1) with the appropriate coefficients. If one considers a more complex process with the multistage deformation, with the static, dynamic and metadynamic recrystallization, with the grain growth not only during the recrystallization, but also after the recrystallization, and concerns with the microstructure, then only the 3D CA can be used whereas it demands more time for the calculation. Only the 3D CA can be used if one try studying the processes connected with the microstructure evolution, because every simplification including dimensions reduction introduce inaccuracies, which can up-end all results.

7. CONCLUSIONS

In the paper four problems are presented, which can either prohibit or hamper the using of the 2D CA. It has been shown that the 2D CA cannot give the proper results for the recrystallization kinetics, the grains sizes, the grain growth rate and the nucleation rate simultaneously. One can receive only one of them, rarely some of them, but not all. An approach to the real results in 2D CA is possible and demands introduction to the CA more complicated algorithm. Modeling by the 2D CA still remains and will be for a while the most popular variant of the CA. But for accurate quantitative calculation by the 2D CA, researchers patience and attention are required to the abovementioned problem (for example, definition of nucleation rate and grain growth rate).

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WYBRANE PRZESŁANKI PODWAŻAJĄCE ZASTOSOWANIE AUTOMATÓW KOMÓRKOWYCH 2D DO MODELOWANIA REKRYSTALIZACJI

Streszczenie

Czas obliczeń jest głównym czynnikiem dającym preferencję zastosowań rozwiązania 2D w porównaniu z 3D. Liczba komórek w przestrzeni 2D jest kwadratem tej przestrzeni, a w 3D jest to trzecia potęga. Zwiększa to również liczbę sąsiadów danej komórki. W konsekwencji czas obliczeń 3D jest dłuższy więcej razy, niż wynikałoby to tylko z rozmiaru przestrzeni. Automaty komórkowe są powszechnie używane do modelowania krystalizacji, rekrystalizacji, przemian fazowych, propagacji pęknięć, rozwoju mikropasm i pasm ścinania itp. Powstaje pytanie czy rozwiązanie 2D może oddać poprawnie realny proces? W artykule opisano pewne aspekty zastosowania rozwiązania 2D do opisu rekrystalizacji. Rozważono cztery problemy, które mogą być rozwiązane lub chociaż przeanalizowane. Są to kinetyka rekrystalizacji, zarodkowanie, wzrost ziaren i odkształcenie ziaren. Niektóre z tych problemów mogą być rozwiązywane tylko dla statycznej rekrystalizacji. W pracy przedstawiono pewne propozycje i rekomendacji w tym zakresie.

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