# Computation of interface curvature in modelling of solidification by the method of cellular automaton

**A.A. Burbelko\*, W. Kapturkiewicz, D. Gurgul**

AGH – University of Science and Technology, Faculty of Foundry Engineering, 23 Reymonta Str., 30-059 Krakow, Poland
\*Mailing address: abur@agh.edu.pl

## Abstract

Modelling of solidification process by the method of cellular automaton (CA) requires determination of geometrical characteristics of the interface, i.e. of its direction and curvature. In previous studies the authors proposed a method to reduce the well-known effect of an artificial symmetry of the simulation results caused by the anisotropy of the CA computation grid (e.g. a preferred growth of the main dendrite arms along the grid lines or at an angle of 45° in the case of grids with square cells). The aim was achieved by application of the developed methods of computation of the transformation rate and front direction. In this study the authors examined the problem of an accuracy of the computations of an interface curvature. The obtained results show us that the error of the curvature computation introduced by some well-known methods exceeds by 100% a nominal value of this parameter. A method to estimate the accuracy of the applied solution has been proposed. Practical application of the proposed tests enables selection of a best solution, including the authors' own solutions, thus considerably improving an accuracy of the solidification modelling by the method of CA.

**Key words:** Solidification Modeling; Cellular Automaton; Artificial Anisotropy

## 1. Introduction

One of the methods used to forecast the microstructure of materials is by modelling the phase transformations and grain growth on cellular automata. In modelling of this type, the shape of crystals and their internal structure (e.g. the radius of the dendrite front curvature, secondary dendrite arm spacing, etc.) are not included in model assumptions, but are determined directly during the simulation.

The cellular automata are an idealisation of a physical system in which space and time are discrete, and the physical quantities take only a finite set of values [1]. In modelling of phase transformations the mathematical tools operating in CA are used to define the state of cells (e.g. "solid", "liquid", "interface"). The well-known and available solutions combine modelling of the interface shape by CA method with modelling of mass and heat

diffusion by the finite difference method on a CA grid. Modelling of this type allows for an effect of the alloy constituents segregation and its influence on changes in the temperature of thermodynamic equilibrium. The value of capillary undercooling related with the interface curvature is also taken into consideration. The capillary undercooling indicates changes in the temperature of the thermodynamic equilibrium on a non-zero curvature surface compared with the flat (zero curvature) surface.

A review of the mathematical models using CA has been presented in [2].

A parabolic differential equation with partial derivatives (also known as diffusion equation or Fourier equation) is used in modelling of the temperature field:

$$c\frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + q_T$$

(1)

and/or in modelling of the concentration field:

$$\frac{\partial C}{\partial \tau} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D \frac{\partial C}{\partial y}\right) + q_C$$

(2)

where:

| | | |
|---|---|---|
| $T$ | – | temperature, |
| $C$ | – | concentration, |
| $\tau$ | – | time, |
| $c$ | – | volumetric heat capacity, |
| $\lambda$ | – | thermal conductivity, |
| $D$ | – | diffusion coefficient, |
| $x, y$ | – | coordinates. |

The functions of source $q_T$ (heat) and $q_C$ (mass) have non-zero values only in these cells of the grid (called interface cells) which cross the interface. The value of these functions is proportional to the interface migration rate. To determine parameters of the vector of the interface movement velocity, it is necessary to determine the geometrical characteristics of the solid/liquid interface, i.e. its position, the direction of normal versor, and curvature.

When the dendritic solidification is an object of the modelling, most of the well-known publications report on the presence of an artificial anisotropy in the results of the simulation, due to the symmetry of the applied grid. According to the results obtained in [3], the structure of the dendrites subject to modelling depends on the grid anisotropy rather than on the properties of the examined constituent. The effect of the grid anisotropy on the structure was also reported in the studies done on modelling of the recrystallization, e.g. [4, 5].

It has been established that most responsible for the significant effect of the grid symmetry on the anisotropy of the results of the dendritic solidification simulation by CA are the methods used currently for determination of the phase transformation rate in the cells of an interface [6] and for determination of the direction of normal versor [7].

Literature states several techniques applicable in computation of the transformation rate [2, 8, 9] and interface direction [8, 10]. In [6, 7] the following tests were proposed to check these methods of computations: *Growth Rate Circle Test* (GRCT) and *Interface Direction Circle Test* (IDCT). The proposed tests are meant to help in selection of the best solution, the authors' own solutions included, to reduce the artificial anisotropy of the simulation results.

In reference literature one can also find a description of different methods used for computation of the interface curvature, and therefore in this study an attempt has been made at developing an *Interface Curvature Test*. The aim of the test is to assist the selection of a most accurate method to be used in determination of this curvature.

# 2. Computation of the interface curvature

## 2.1. The well-known methods of the computation of surface curvature

The well-known techniques used for the computation of surface curvature can be divided into three groups: counting-cell technique [11, 12], differential technique [13], and geometric technique [2].

In the counting-cell technique (CCT) it is assumed that the curvature is proportional to a difference between the actual number of the cells of the transformed phase in the examined neighbourhood ($N_s$) and the number of such cells on a planar front ($N_{pl}$) [11]:

$$\kappa = \frac{2}{a}\frac{N_{pl} - N_s}{N_t}$$

(3)

where:

| | | |
|---|---|---|
| $N_t$ | – | total number of cells in the examined neighbourhood; |
| $a$ | – | cell size. |

In the differential method (DM), the line curvature is determined from space derivatives. The interface curvature equals the divergence of a normalised gradient of function $F(x,y)$, describing the distribution of solid fraction in the examined neighbourhood [14]. In [10, 12] for computation of the curvature, the following equation was used:

$$\kappa = \left(2F_{xy}F_x F_y - F_{xx}F_y^2 - F_{yy}F_x^2\right)\left(F_x^2 + F_y^2\right)^{-3/2}$$

(4)

where subscripts denote the differentiation done on the respective variables.

Geometric method (GM) uses the flat line curvature definition as a limit for the quotient of a change of normal vector direction at the end points on the line segment ($\Delta\theta$) divided by the length of this segment ($\Delta s$):

$$\kappa = \Delta\theta / \Delta s$$

(5)

## 2.2. Interface Curvature Circle Test

The task of the first test is to estimate if the curvature has been computed in a correct way. In this test based on GRCT [6] it has been assumed that the grain growth velocity is constant and independent of the growth direction. For each cell of an interface the direction of the velocity vector is determined by a line joining the centre of this cell with the centre of the nucleus. The angle $\theta$ between the reference direction and the velocity vector depends only on the coordinates of the cell centre:

$$\theta = arctg \frac{i - i_N}{j - j_N} \qquad (6)$$

where:

$i, j$ — indeces of the interface cell;
$i_N, j_N$ — indeces of the cell-nucleus.

The initial radius of the nucleus is equal to the length of the side of a cell in the CA grid ($a$). The growth velocity has been chosen so as to make the grain radius $r$ increase by 1% of the value $a$ at each time step $\Delta\tau$:

$$u = \frac{0.01a}{\Delta\tau} \qquad (7)$$

The change in the solid phase fraction was computed from an equation which ensures that the growing grain will preserve its isotropic shape [6]:

$$\Delta f = \frac{\Delta\tau}{a} \frac{u}{|\cos\theta| + |\sin\theta|} \qquad (8)$$

The accuracy of computations of the interface curvature by means of equations (1) – CCT, (2) – DM and (3) – GM was estimated qualitatively from the graphs illustrating a deviation from the nominal curvature of the curvature computed for individual interface cells on the grain perimeter.

The results of the test are shown in a dimensionless form in Figure 1 (as a length unit is used the length of a side of the CA grid cell). In computation of the curvature by means of CCT the environment of 3x3 AC cells has been used. In computation of the curvature by the differential method, the technique of interpolation of the field of the product fraction after transformation described in [15] has been used. The details of the geometric method used for computation of the interface curvature are presented in [2].

The curvature computed by CCT (Fig. 1a) is characterised by the scatter of results smaller than DM (Fig. 1b), but for small radii (typical of the dendritic front) it is burdened with a large systematic error. A maximum accuracy of the determination of a mean value of the curvature as well as a minimum scatter of the results are offered by the geometric method (Fig. 1c).

## 2.3. Interface Curvature Kinetic Test

The second of the proposed tests allows for an effect of the tested method on the correct modelling of the growing grain shape, taking into account the temperature field and capillary undercooling as well as its effect on the rate of transformation. In computations, a mathematical model of solidification described in [2] was used.

Testing of model equations was carried out on a square CA 200×200 cells lattice of the side length $a = 1$ μm. The nucleus of

an initial radius equal to the side length of a cell in the CA grid was placed in the centre of the computation grid. The adopted initial value of temperature within the simulated area was:

$$T_0 = T_M - 0.01\frac{L}{c} - 1, \text{K} \qquad (9)$$

where:

$T_M$ — melting temperature;
$L$ — solidification heat;
$c$ — specific heat.

To eliminate the anisotropy of temperature field imposed by the square shape of the grid, a first-type boundary condition ($T=T_0$) was introduced to the grid cells distant from the grain centre by a section larger than $100 \cdot a$.

In the test, besides the heat flow, also the effect of capillary undercooling on the transformation rate and precipitation of the solidification heat was taken into account. The adopted value of Gibbs-Thomson coefficient was assumed to be equal to:

$$\Gamma = \frac{0.01 \cdot a \cdot L}{c} \qquad (10)$$

Under such assumptions, the kinetic undercooling was of the same order of magnitude as that of the capillary undercooling computed from the following equation:

$$\Delta T_\kappa = \Gamma \cdot \kappa \qquad (11)$$

This is why the shape of the growing grain was sensitive to an inaccuracy of the computation of local curvature. The same material constants as for the Fe-C alloy were selected:

- liquidus temperature $T_M = 1673$ K,
- heat of solidification $L = 1.97 \cdot 10^9$ J/m$^3$,
- specific heat $c = 5.84 \cdot 10^6$ J/K·m$^3$,
- heat conductivity $\lambda = 30$ W/K·m.

Figure 2 shows the results of computations of a mean curvature on the perimeter of the growing grain (the thick black line) and of a standard deviation of this value (thin line) as obtained by the *Interface Curvature Kinetic Test*. The thick grey line in this drawing shows a nominal value of the curvature computed from the following equation:

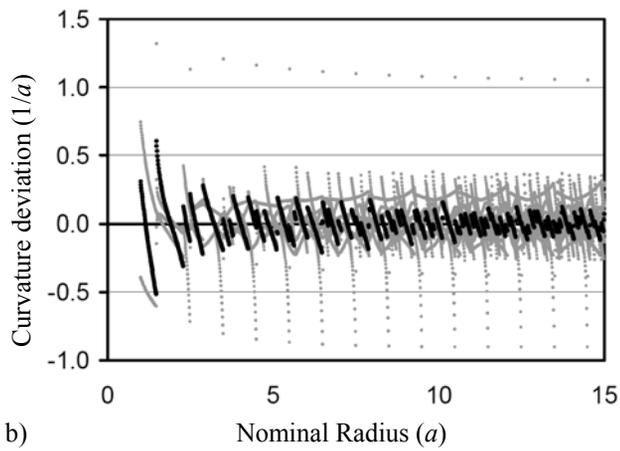$$K_n = \sqrt{\frac{\pi}{\sum_{i,j} f_{i,j}}} \qquad (12)$$

where:

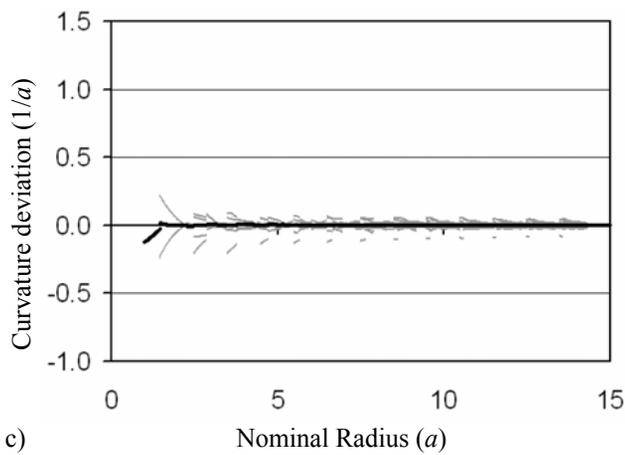$f_{i,j}$ — fraction of the transformation product in grid cell ($i,j$).

From this drawing it follows that the use of CCT (Fig. 2a) gives a significant underestimation of the surface curvature of the growing grain. The value of standard deviation is comparable with the mean values, which also indicates a large scatter of the data in respect of the mean.
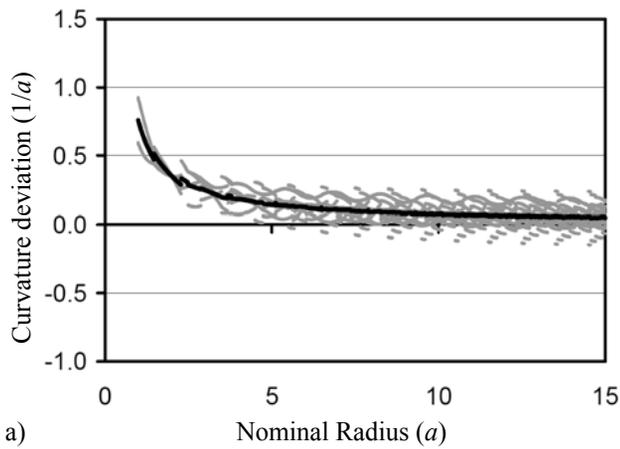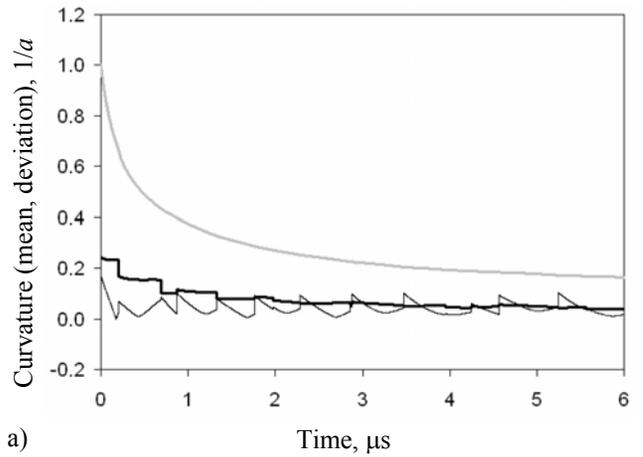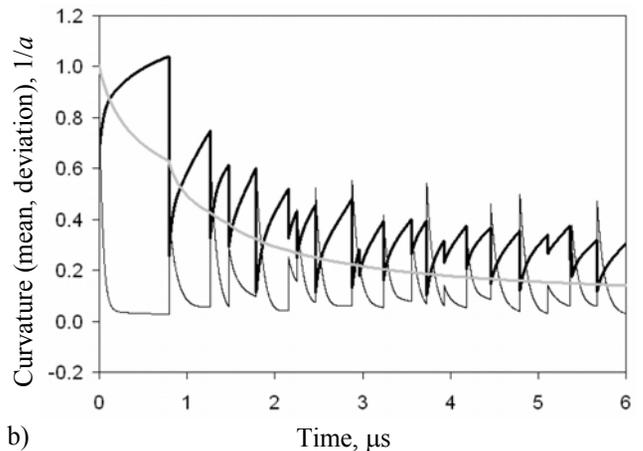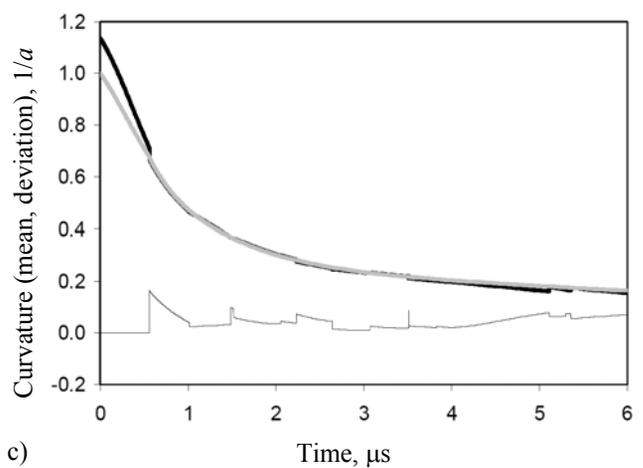
Fig. 1. The results of *Interface Curvature Circle Test*: a) CCT, b) DM, c) GM (black – mean value)



Fig. 2. The results of *Interface Curvature Kinetic Test*: a) CCT, b) DM, c) GM (thick black line – mean curvature obtained in the test; thin line – standard deviation of the curvature on grain perimeter, thick grey line – nominal curvature)
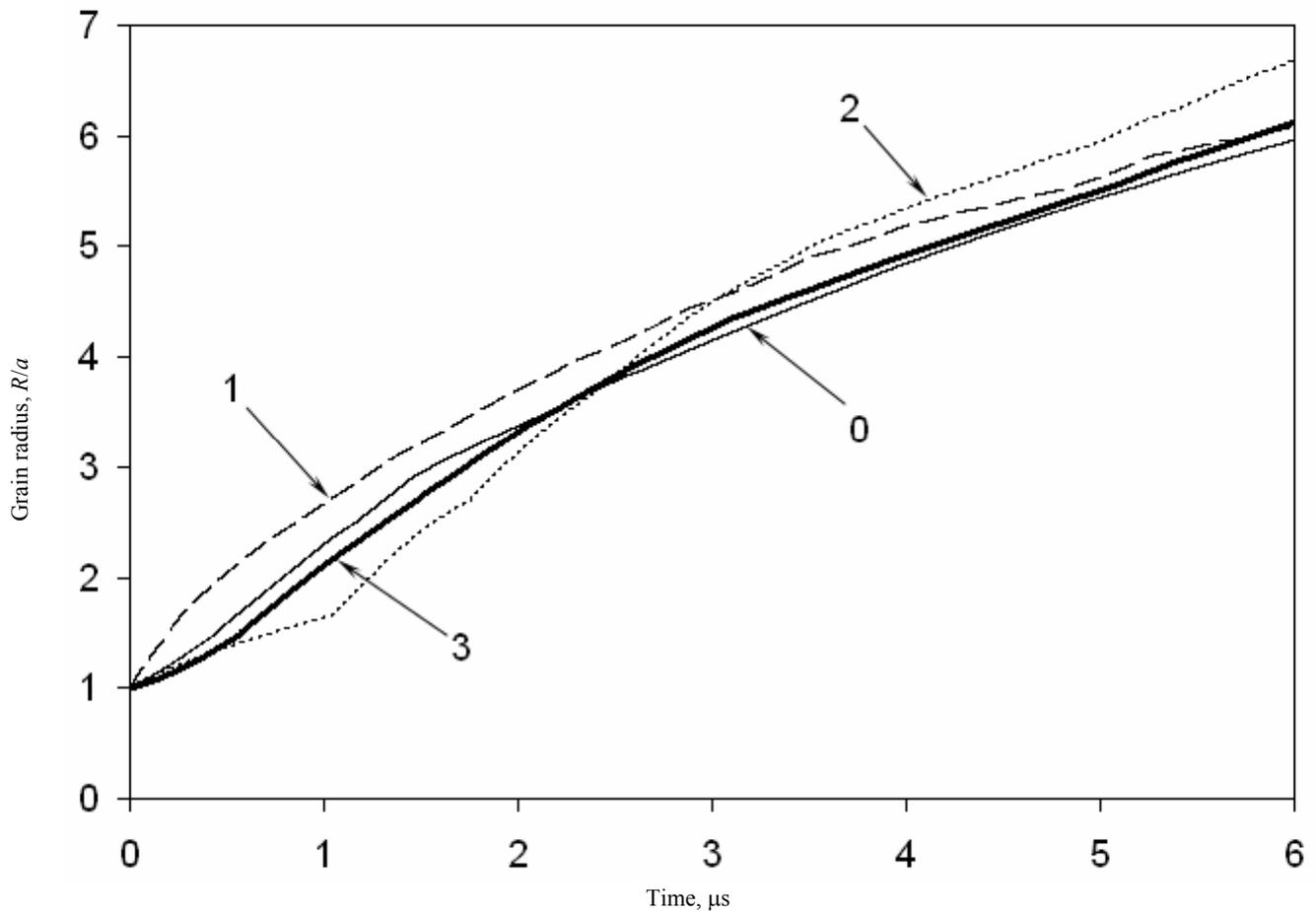
Fig. 3. Results of *Interface Curvature Kinetic Test*: 0 – reference curve, 1 – CCT, 2 – DM, 3– GM

When the differential method is used (Fig. 2b), large deviations of the mean test result from the nominal value of the curvature are observed to occur periodically with prevalence of the positive deviations. Compared with the methods described previously, the geometric method (Fig. 2c) gives but only a minimum positive deviation of the computed curvature from the nominal value and is characterised by a minimum and stable level of the standard deviation.

Figure 3 shows the kinetics of changes in the grain radius during *Interface Curvature Kinetic Test*. The reference curve (line 0) in this drawing was plotted by numerical modelling under the assumption that the solidification front curvature in individual cells of the interface equals the nominal value computed from equation (10).

From this drawing it follows that, compared with the reference line (line 1), the underestimated curvature in the case of CCT results in an overestimated grain growth velocity. The use of differential method (line 2) initially retards the grain growth to accelerate it after some 2.5 µs. The use of geometric method (line 3) gives the best consistency between the grain radius computed in tests and the reference values.

## 3. Conclusions

A test has been developed by means of which it is possible to evaluate the accuracy of computations of the interface curvature in modelling of solidification by the technique of cellular automaton.

By means of this test it has been proved that the most accurate technique of computation of the interface curvature in mathematical modelling of the solidification on CA is the geometric method using equation (3).

## Acknowledgments

# Literature

[1] B. Chopard, M. Droz, Cellular automata modeling of physical systems. University Press, Cambridge, 2005.

[2] A. Burbelko, Mezomodeling of Solidification Using a Cellular Automaton, AGH, Kraków, 2004 (in Polish).

[3] M. Rappaz, Ch.-A.Gandin, A. Jacot, Ch. Charbon, Modeling of microstructure formation, Modeling of Casting, Welding and Advanced Solidification Processes – VII, TMS, Warrendale, 1995, 501–516.

[4] J. Kroc, Influence of Lattice Anisotropy on Models Formulated by Cellular Automata in Presence of Grain Boundary Movement: A Case Study, Mat. Sci. Forum, vol. 482 (2005), 195–198.

[5] Y.J. Lan, D.Z. Li, Y.Y. Li, A Mesoscale Cellular Automaton Model for Curvature-Driven Grain Growth. Met. and Mater. Trans. B, vol. 37B (2006), 119–129.

[6] A.A. Burbelko, D. Gurgul: Testing of the Growth Rate Governing Equations for Cellular Automata Solidification Modeling. Simulation, Design and Control of Foundry Processes. AGH, Kraków, 2006, 21-32.

[7] A.A. Burbelko, W. Kapturkiewicz, D. Gurgul, Problem of the artificial anisotropy in solidification modeling by cellular automata method. Computer Methods in Materials Science. no. 1, vol. 7 (2007), 182-188.

[8] U. Dilthey, V. Pavlik, Numerical simulation of dendrite morphology and grain growth with modified cellular automata, Modeling of Casting, Welding and Advanced Solidification Processes VIII. TMS, Warrendale, 1998, 589-596.

[9] M.F. Zhu, C.P. Hong, A modified cellular automation model for the simulation of dendritic growth in solidification of alloys. ISIJ International, no 5, vol. 41 (2001), 436-445.

[10] L. Beltran-Sanchez, D.M. Stefanescu, A quantitative dendrite growth model and analysis of stability concepts. Met. and Mater. Trans. A, no. 8, vol. 35A (2004), 2471–2485.

[11] R. Sasikumar, R. Sreenivasan, Two dimensional simulation of dendrite morphology, Acta Metall. Mater, vol. 42 (1994), 2381-2386.

[12] L. Nastac, Numerical modeling of solidification morphologies and segregation patterns in cast dendritic alloys. Acta Mater., vol. 47 (1999), 4253-4262.

[13] R.A. Umancev, V.V. Vinogradov, V.T. Borisov, Matematićeskoje modelirovanieje rosta dendritov v pere–ohlazh–dennom rasplave, Kristallografija, vol. 30 (1985), 455-460 (in Russian).

[14] S. Osher, R.P. Fedkiw, Level Set Methods: An Overview and Some Recent Results. Journal of Computational Physics, vol. 169 (2001), 463-502.

[15] M. Marek, Dendritic Solidification Modeling in the Areas with a Stable Heat Condition with CA Using, Ph.H.D Thesis, PCz, Częstochowa (2006) (in Polish).