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SYSTEM PARAMETERS INVESTIGATION FOR STEFAN PROBLEM SOLVING BY THE CONTINUOUS ASYNCHRONOUS CELLULAR AUTOMATA METHOD

The main object of this work is to construct a cellular automaton (CA) model of heat conductivity processes with first order phase transitions. The paper discusses main approaches and general methodology for development of cellular automata models. The studies were conducted on the example of cellular automata to model moving phase boundary problems for freezing of moist soil, the process of band Bi2Te3 growing and changing forms of solidification front. It is shown that the CA models can be an alternative to the use of classical differential equations. It is proven that the model as a system of cellular automata is quite a convenient tool for the study of nonlinear heat transfer problems, despite the simplicity of its description, and may describe very complex system behaviour.

Key words: *first order phase transition, cellular automata, thermal conductivity, Stefan problem, zone growing.*

Introduction

The matter of solving heat conductivity problems is quite important, especially for cases with non-linear parameters of materials. For the majority of these problems, a numerical solution is a common approach. But when it comes to systems with complex boundary conditions or phase transitions of the substance, the computational complexity makes us look for alternative methods. Cellular automata algorithm easily describes such complex systems.

1. Related works

In recent years, alternative approaches to numerical methods for problems of heat conductivity and diffusion are widely used. Cellular automata algorithms are quite successfully used [1, p. 58; 2, p. 497] for this purpose. It should be noted that discrete models are used in most cases for calculation of diffusion processes [3, p. 1019], and continuous models of cellular automata [4, p. 127; 5, p. 266] are used to approximate heat transfer processes.

A lot of attention of researchers in the field of solid state physics is directed towards the study of problem of structural parameters of real materials with different physical nature and different spatial dimensions. In such cases, it makes sense to use modelling techniques that easily describe complexity of system geometry [1, p. 69]. Cellular automata simulation has this property. The purpose of this paper is to develop a model of continuous cellular automata and use it to describe the processes of heat conductivity complicated by a first order phase transition.

2. Cellular Automata Model Description

The description of systems with complex boundary conditions or phase transition is in many cases difficult. This is due to the fact that a numerical solution of this problem is quite difficult to obtain because of the large number of calculations.

An example is the problem of describing such complex phenomena as evolution and self-organization, diffusion and thermal conductivity. Let us consider the last process, complicating it by first order phase transition. This task belongs to the class of so-called Stefan problems.

Mathematical formulation of Stefan problem for a three-dimensional case is:

$$\frac{\partial T_S(x, y, z, t)}{\partial t} = a_S \Delta T_S(x, y, z, t)\; a_S = \frac{k_S}{c_S \rho_S}, \qquad (1)$$

$$\frac{\partial T_L(x,y,z,t)}{\partial t} = a_L \Delta T_L(x,y,z,t),\ a_L = \frac{k_L}{c_L \rho_L}, \quad (2)$$

$$\left|k_S \nabla T_S(x,y,z,t) - k_L \nabla T_L(x,y,z,t)\right| = \left|H_f \rho_{(L/S)} \frac{d\xi}{dt}\right|, \quad (3)$$

where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$;– the Laplace operator; $\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$ – the Hamiltonian operator; T_S and T_L, a_S and a_L, k_S and k_L, c_S and c_L, ρ_S and ρ_L – accordingly: temperature, thermal diffusivity, thermal conductivity, specific heat capacity, specific density of the solid and liquid phases; Hf – latent heat of fusion; ξ – coordinate of the interface of two phases. Specific density symbol $\rho_{(L/S)}$ on the right side of equation (3) means that the corresponding value of liquid /solid phase is selected depending on the direction of the phase transition – crystallisation /melting.

Heat conduction, described by the equation (1)-(3) may be modelled by cellular automata method. But for organizations quantitative calculations it is necessary to answer the question how much you should make cellular automata interactions for the resulting temperature distribution could be considered as solution of the problem in time t.

The essence of modeling of heat conduction using cellular automata is as follows. We partition the sample into a plurality of identical the same way interconnected cells. All cells form the so-called lattice cellular automaton. Lattices may be of different dimensions (the one-, two-or three-dimensional array), depending on the dimension of the modelled system.

In the case of modeling complex phenomena involving phase transitions or other changes, the contents of the cells of cellular automata field may be a single linear array of certain characteristics of the cell which, in turn, except temperature (for modeling thermal conductivity) and concentration (for diffusion processes) may contain some other parameters, such as the index of the state of matter, the internal energy and the like.

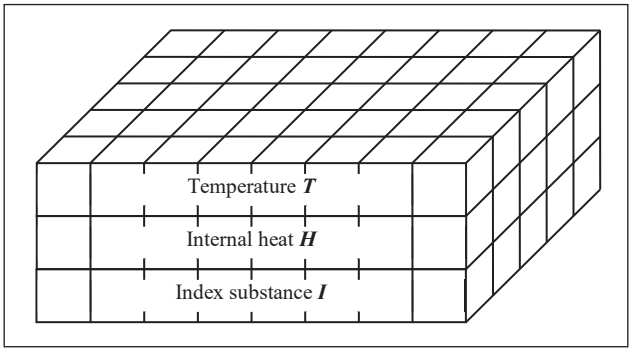

Fig. 1. Structure of the cellular automata field for a two-dimensional model

Consider, for clarity, two-dimensional field CA (Fig. 1), which contains three layers: 1 – temperature of T cells, 2 – H internal heat, which takes into account in the modeling of phase transitions, 3 – index substance I (or states of matter, such as monocrystal, polycrystal, melt) which is taken into account when selecting the values of the coefficients of thermal conductivity, specific heat and density in the corresponding point of the system. The cell contents of the field can make the real continuous values.

Area of the cell is determined by the dimension of the field of cellular automata, in accordance with the geometrical dimensions of the fragment of the simulated system.

Cellular automata can be realized in different ways. In this paper we use asynchronous scheme of interactions of cellular automata, providing cyclic execution of three typical steps:

1. Some cell $i = 1$ with integer coordinates x_1, y_1 is selected randomly on a cellular automata field.

2. A neighbouring cell $i = 2$ with integer coordinates x_2, y_2 is selected in an equiprobable way. The Neumann neighbourhood is accepted as a neighbourhood scheme in this case, i.e. a cell has only four neighbours.

3. A cellular automata interaction between the two cells takes place.

The described method of continuous asynchronous cellular automata can be applied to solve problems of heat conduction. In particular, it is shown in [6, p. 97].

The essence of cellular automata interactions is to modify the values of corresponding continuous layers of cells according to the following system of equations:

$$\begin{cases} T^{i'} = T^i + (T_m - T^i) a_m / a_{max}; \\ \text{if } (T^{i'} > T_f) \text{ and } (H^i < H_f), \text{ then } \{H^{i'} = H^i + c_S^i (T^{i'} - T_f); T^{i'} = T_f;\} \\ \text{if } (H^{i'} > H_f), \text{ then } \{T^{i'} = T^{i'} + (H^{i'} - H_f)/c_L^i; H^{i'} = H_f;\} \\ \text{if } (T^{i'} < T_f) \text{ and } (H^i > 0), \text{ then } \{H^{i'} = H^i + c_L^i (T^{i'} - T_f); T^{i'} = T_f;\} \\ \text{if } (H^{i'} < 0), \text{ then } \{T^{i'} = T^{i'} + H^{i'}/c_S^i; H^{i'} = 0;\} \end{cases}$$

$$a_m = (a^1 + a^2)/2,\ a^i = k^i / \rho^i c^i,\ T_m = \frac{w^1 T^1 + w^2 T^2}{w^1 + w^2},\ w^i = \rho^i c^i, \quad (4)$$

where a – thermal diffusivity $i = 1, 2$ – index value that corresponds to the selected cell and the adjacent cell with coordinates (x^1, y^1) and (x^2, y^2) respectively. Values at the next moment are stroke-marked.

The first equation of system (4) is a cellular automaton analogue of the heat equation (1) and (2) which has been investigated in [7, p. 294], the rest of the equation in (4) – approximation of equation (3), the

second and third equations of system (4) describes the process of melting, and the fourth and fifth – the process of crystallization.

The system of equations (4) describes the change of temperature and latent melting heat of the respective cells during one elementary interaction of cellular automata. It is a kind of Stefan problem numerical solution approximation (1–3).

3. Calculation Results Analysis

It is necessary to define the parameters accuracy of the approximation depend on and their influence on it. This will prove as viable modeling of heat conduction by cellular automata method.

For simplicity, consider a one-dimensional homogeneous sample [7, p. 297]. We will take the coefficients of thermal diffusivity equal to a constant. (1) becomes in this case:

$$\frac{\partial T(x,t)}{\partial t} = a\frac{\partial T^2(x,t)}{\partial x^2},\ a = \frac{k}{c\rho}, \qquad (5)$$

From solution of the equation (5), in the area of substance with length d comes up some value – the characteristic time of establishing of the temperature in the system:

$$t_{est} = \frac{d^2}{a}, \qquad (6)$$

We try to estimate the time of single cellular automata interaction for described above asynchronous approach. We assume $d = 1$, $a = 1$. Then the characteristic size of a single cell $d \sim 1/N$, where N – number of cells cellular automata field. On the other hand, the probability of selection of cells for the interaction act as equals $1/N$. That is to provide a choice of given cell it should be implemented in the average N sampling from the total population. By analogy with the process of mass transfer in the diffusion, where the diffusion coefficient is directly proportional to the number of elementary acts of mass transfer per unit time we obtain $a \sim N$. Using (6), we obtain:

$$t_{CA} \sim \frac{1}{N^3}, \qquad (7)$$

Confirmation of the statement (7) is possible by means of computer simulation, which consists in comparing the cellular automaton dynamics with different numbers of cells of cellular automata field with a particular solution of equation (5). Based on this experiment, temperature distribution $T(x,t)$ was constructed in a range $x \in [0,1]$ in different time points.

In parallel with calculations was performed the cellular automata simulation of the heat transfer. In cases where the maximum similarity, which was analyzed by the method of least squares on the set of control points, was fixed number of cellular automata interactions.

By analyzing results of computational experiments it is possible to confirm the validity of relation (7), as well as get a proportionality factor.

Thus, time of a cellular automata interactions for the described method is for three-dimensional model ($N_x \times N_y \times N_z$):

$$t_{CA} = \frac{d_x^2}{a_{\max}}\frac{1}{6N_x^3N_yN_z} = \frac{d_y^2}{a_{\max}}\frac{1}{6N_y^3N_xN_z} = \frac{d_z^2}{a_{\max}}\frac{1}{6N_z^3N_yN_x}, \qquad (8)$$

where d_x, d_y, and d_z – the dimensions of the sample along coordinate x, y and z, respectively.

At figure 2 is shows a high degree of coincidence of solutions, which confirms the adequacy of the use of cellular automata approach for approximation of the solution of nonstationary heat conduction equation.

From the foregoing it can be concluded that the dimension of cellular automata field must be as large

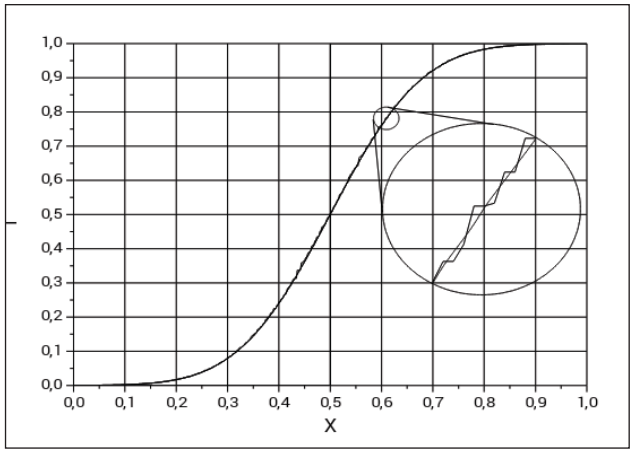

Fig. 2. Temperature distribution in the sample at time t = 0,01s (N = 500). Smooth line - decision by the formula (5), broken - cellular automata decision

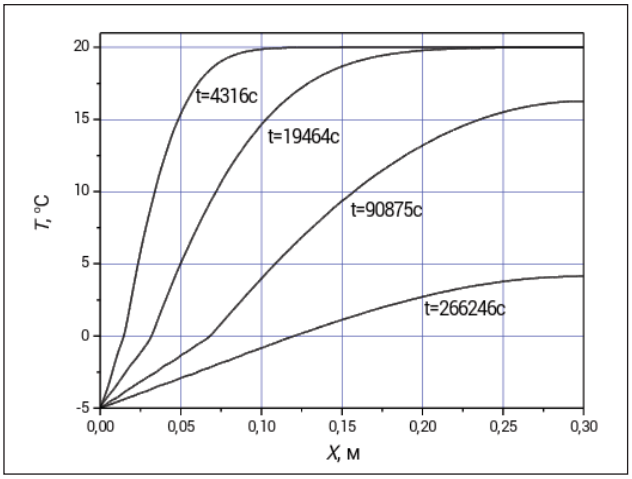

Fig. 3. Temperature distribution over the depth of the soil

as possible to ensure the adequacy of the modeling process. On the other hand, it will necessarily lead to long-term modeling process. Therefore, it is need to look for compromise between the accuracy of the solution and the time required to obtain it to solve this problem. With this shortcoming of the proposed method it can be overcome by using parallel computing [8, p. 341], since their principles apply to cellular automata and can significantly increase the size of the model.

By drawing an analogy between the CA method and Monte Carlo simulation, it is easy to notice a similar relationship – the longer the computation time, the more accurate the result. Herewith, as in the case of proposed probabilistic scheme of asynchronous sampling of cellular automata, use of probabilistic mechanisms also takes place in the Monte Carlo method. But unlike the Monte Carlo method for solving equations, cellular automata method is a method of simulation and it can be used to model systems that can not be described in terms of theory of differential equations [1, p. 93].

Further improvement of the proposed cellular automata method results in a need to consider the processes of thermal conductivity, accompanied by first order phase transitions. Let's proceed to consider a non-stationary task of the process of thermal conductivity with first order phase transition i.e., the Stefan problem – freezing of moist soil. Let the moist ground is in thawed state. At the initial moment t = 0 it has a uniform temperature T=20 ° C. Also on the soil surface at the initial moment temperature is instantly set below the freezing point T = -5 ° C. As a result, there will be a freezing. Formed frozen layer will have a variable thickness $\xi = f(t)$. Its movable boundary always has a freezing point. At this boundary take place transition from one state to another, which takes the heat of transition H_f, (J/kg). Thus, the boundary $x = \xi$ of the melt zone has a constant freezing temperature and the thermal conditions on the boundary $x = L$ we assume adiabatic. Assume the depth of soil equal to L = 0,3 m. Calculations of temperature distributions in the depth of the soil were performed at various time points by using the cellular automata approach. The results of calculations for one-dimensional (N_x = 500), two-dimensional ($N_x \times N_y$ = 500×100) and three-dimensional ($N_x \times N_y \times N_z$ = 500×10×10) CA models along the x axis are shown in Fig.3.

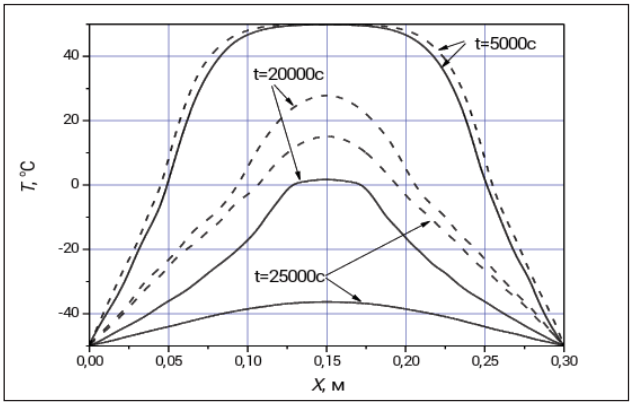

Fig. 4. Temperature distribution along the diagonal section of the cylinder (solid line) and along the cross section of the square bar (dotted lines)

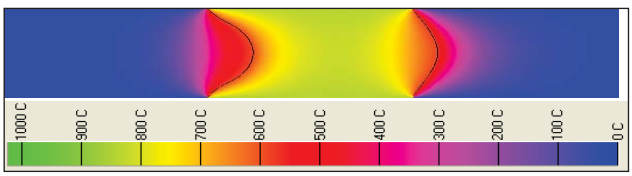

Fig. 5. Example of simulation of a zone growing Bi_2Te_3

Models of different dimensions agree with one another and with the corresponding results of numerical solutions of equations (1) – (3) for a given problem of freezing of moist soil [6, p. 35].

Another example of the Stefan problem was examined in this paper. The process of zone growing of materials was modelled on the example of bismuth telluride (Bi_2Te_3). In practice, zone growing of materials often occurs in cylindrical quartz ampoules. For realization of cellular automaton model of the growth process, the cylindrical symmetry of the system (by including the multiplier $(1 + \pi R)$ in (4) for weight coefficient) was taken into account, which made it possible to reduce a three-dimensional model to a two-dimensional one and by that reduce the computing time with other parameters of the model being constant. So the expression becomes: $w^i = \rho^i c^i \left(1 + \pi R^i\right)$ where R^i – the distance from the axis of the cylinder to the i-th cell. Please note that the parameters a_m, a_{max}, t_{1CA}, H_f does not depend on the multiplier, since the thermal parameters of the material does not change. To test our hypothesis, execute the computational experiments to cool square-section bar $D \times D$ and cylinder of diameter D. Significant discrepancies for the distribution of temperature of the bar and the cylinder in different times are shown at Fig. 4. But solutions completely coincide if we consider the multiplier.

Thus it is possible to realize a two-dimensional cellular automata model of zone growing materials in cylindrically symmetric quartz ampoules. An example of modelling the process of growing zone Bi_2Te_3 is shown at Fig. 5. Parameters that provide a flat crystallization front have also been obtained and empirically confirmed [7, p. 298]. Their receipt

ensured uniformity of physical parameters along the cross-section of the ingots. Equality of real and model growth parameters, in which there is a flat crystallization front [7, p. 300] demonstrates the adequacy of the described cellular automata approach.

Conclusion. Cellular automata model that describes the processes of thermal conductivity, accompanied by first order phase transitions was also presented. Parameters that provide the plane crystallization front in itinerant growing of semiconductor materials and the temperature distribution along the depth of the soil at different times moments for problem of freezing of moist soil were obtained and empirically validated.

As a conclusion, we note that the proposed method can be a worthy alternative to the previously known classical methods of Stefan problems solving and has prospects due to its versatility and simplicity. It implies that the method of continuous cellular automata can be used for description of dependence of the phase transition temperature on composition and modelling of instability of crystallization front.

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ДОСЛІДЖЕННЯ ПАРАМЕТРІВ СИСТЕМИ ДЛЯ ВИРІШЕННЯ ЗАДАЧІ СТЕФАНА ЗА ДОПОМОГОЮ МЕТОДУ АСИНХРОННИХ КЛІТИННИХ АВТОМАТІВ

Стаття присвячена побудові клітинно-автоматної моделі (КА) процесів теплопровідності з фазовими переходами першого роду. У роботі розглянуто основні підходи та загальну методологію розробки клітинно-автоматних моделей. Дослідження проводилися методом клітинних автоматів для моделювання задач із рухомим фронтом розділу фаз на прикладі задачі промерзання вологого ґрунту та зміни форм фронту кристалізаії в процесі вирощування Bi2Te3. Показано, що КА-моделі можуть бути альтернативою використанню класичних диференціальних рівнянь. Доведено, що модель як система клітинних автоматів є досить зручним інструментом для вивчення нелінійних задач теплопровідності, незважаючи на простоту її опису, і може описувати дуже складну поведінку системи.

Ключові слова: *фазовий перехід першого роду, клітинний автомат, теплопровідність, задача Стефана, зонне вирощування.*

ИССЛЕДОВАНИЕ ПАРАМЕТРОВ СИСТЕМЫ ДЛЯ РЕШЕНИЯ ЗАДАЧИ СТЕФАНА С ПОМОЩЬЮ МЕТОДА АСИНХРОННЫХ КЛЕТОЧНЫХ АВТОМАТОВ

Статья посвящена построению клеточно-автоматной модели (КА) процессов теплопроводности с фазовыми переходами первого рода. В работе рассмотрены основные подходы и общая методология разработки клеточно-автоматных моделей. Исследования проводились методом клеточных автоматов для моделирования задач с подвижным фронтом раздела фаз на примере задачи промерзания влажного грунта и изменения форм фронта кристализаши в процессе выращивания Bи2Te3. Показано, что КА-модели могут быть альтернативой использованию классических дифференциальных уравнений. Доказано, что модель как система клеточных автоматов является достаточно удобным инструментом для изучения нелинейных задач теплопроводности, несмотря на простоту ее описания, и может описывать очень сложное поведение системы.

Ключевые слова: *фазовый переход первого рода, клеточный автомат, теплопроводность, задача Стефана, зонное выращивание.*