Thermodynamic Fundamentals of Cellular Automata Model of the Process of Solidification of Metals and Alloys Considering the Phase Transition

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Abstract

We considered the mathematical apparatus that can be used to calculate the thermal problem associated with the features of solidification of metals and alloys. Thermodynamic laws are presented, that made it possible to correctly take into account the phase transition, a feature of which is to release latent heat. A one-dimensional problem and its generalization to a cylindrical coordinate system are considered.

Keywords

Cellular automata, thermodynamic model, temperature, amount of liquid phase, solidification, phase transition

1. Introduction

In industrial process control systems, including foundries, embedded systems based on microcontrollers are widely used. Unfortunately, direct simulation on microcontrollers is impossible due to limited computing resources. Using cellular automata approach allows simplified calculations on embedded systems.

Description of real metallurgical processes associated with solidification [1, 2] leads to significant differences from the classical boundary value problem due to many factors [3, 4], the most important of which are due to: heat release during the phase transition [5], which is described by a complex diagram states [6]; heat transfer due to convective flows in the liquid phase [7, 8]; taking into account the real boundary conditions of heat transfer [9]; inhomogeneity of alloy properties [10, 11]; the dependence of thermophysical parameters on temperature [12]; the complexity of the geometry of the product [13, 14].

The analysis of methods for modelling metallurgical processes showed that the existing analytical solutions of the solidification problem provide a high accuracy of the solution [15, 16], but can be used only in some simple cases and are rather methodological in nature [17, 18]. The description of the solidification problem in the form of partial differential equations leads to the use of numerical solution methods [19, 20], for which a wide range of modifications has been developed [19]. They are united by the presence of artificial methods, such as catching

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the front at the grid node, straightening the fronts, successively approximating the position of the transition phase, smoothing the phase transition, introducing the effective heat capacity [21] and then determining the boundaries of the two-phase zone by interpolation, which lead to a distortion of the original physical setting of the considered problem [22, 23, 24]. The use of thermodynamic models [25] presupposes the existence of a large-scale database of experimental data [26] on the redistribution of components between phases, the dependence of the composition and number of precipitated phases on temperature changes under conditions of equilibrium and nonequilibrium crystallization [27].

Thus, the development of mathematical models of metallurgical processes with phase transitions is an urgent task, which is caused by the necessity of improvements of the quality of products of metallurgical production [28, 29, 30] and their cost reduction [31, 32]. The use of cellular automata in the development of mathematical models of solidification [33, 34, 35] makes it possible to describe various nonlinear processes immediately in a discrete language [36, 37] and has a number of advantages associated with the possibility of organizing high-speed parallel computations [38, 39, 40], the obviousness of algorithms, the possibility of using them to describe processes that are difficult or even impossible to describe by partial differential equations.

2. Cellular automata solidification model

Solidification of metals and alloys is accompanied by complex physical and chemical processes in the melt. The most important of them are due to: heat release during the phase transition; heat transfer due to convective flows in the liquid phase; the complexity of the real boundary conditions of heat transfer; heterogeneity of alloy properties; dependence of thermophysical parameters on temperature; the complexity of the geometry of the product [41].

Thermodynamic phenomena accompanying the process of solidification of metals is described by the Fourier equation [42]

$$\triangle Q = \frac{kS \triangle T}{h}\tau, \tag{1}$$

where $\triangle Q\,[J]$ – the amount of heat passed through the surface $S\left[m^2\right]$ for the time $\tau\,[s]$ with temperature differences $\triangle T\,[K]$, $k\,[W/(mK)]$ – – coefficient of thermal conductivity, $h\,[m]$ – layer thickness.

Equilibrium Specific Energy $q\,[J/kg]$ is uniquely related to the temperature and phase state of the unit volume

$$q = \frac{Q}{\rho h S}, \tag{2}$$

where $\rho\left[kg/cm^3\right]$ – density.

2.1. One-dimensional cellular automata thermodynamic model

The cellular automaton mathematical model assumes the description of nonlinear processes in a discrete language at once and allows avoiding the description of thermodynamic processes in

the form of partial differential equations [43].

To construct a one-dimensional thermodynamic model of solidification, taking into account the phase transition, it is necessary to determine the rules of heat transfer between cells. Consider a cell with a Neumann neighbourhood for the one-dimensional case (Fig. 1).

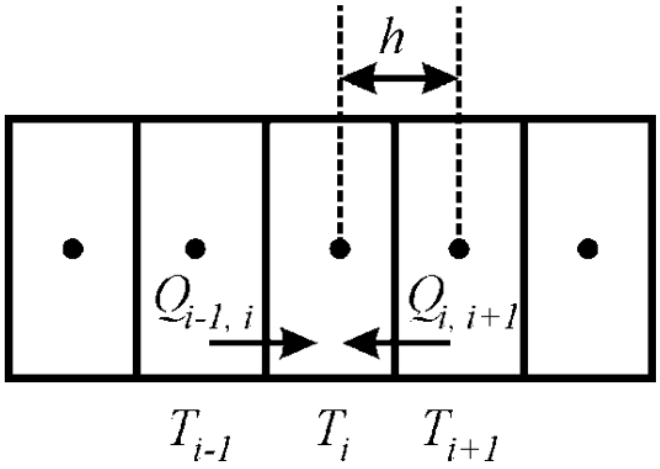

Figure 1: Schematic representation of a group of cells and symbols for the one-dimensional case

Fig. 1 notation accepted: T_{i-1}, T_i, T_{i+1} – temperatures in $i-1$, i, $i+1$ adjacent cells, respectively, h – distance between cell centers, $Q_{i-1,i}$, $Q_{i+1,i}$ – energy entering the cell from $i-1$ and $i+1$ respectively.

Energy entering the cell i from $i-1$ cell, is determined based on the replacement in (1) of the differential by the difference

$$Q_{i-1,i} = \frac{k_{i,i-1} S (T_{i-1} - T_i) \tau}{h}, \tag{3}$$

where $k_{i,i-1}$ – effective coefficient of thermal conductivity, determined from the equality of heat flows at the border of neighboring cells.

A schematic representation of the heat flow motion for the one-dimensional case is shown on Fig.2.

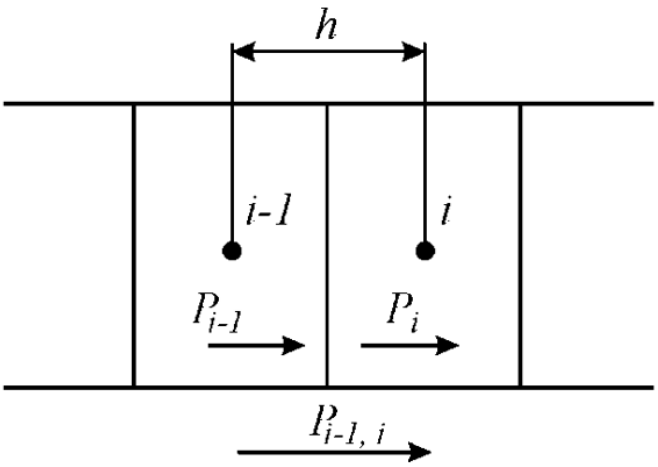

Figure 2: Diagram of heat flow movement between cells

Heat flow $P\,[J/s]$ (fig. 2), corresponding to the amount of energy transmitted through the isothermal surface per unit of time is determined by the ratio

$$P = \frac{kST}{h}. \tag{4}$$

Heat flow between i and $i-1$ cells is equal to

$$P_{i-1,i} = \frac{k_{i-1,i}S(T_i - T_{i-1})}{h}.$$

Heat flow to the border that separates cells:

- from $i-1$ side
$$P_{i-1} = \frac{k_{i-1}S(T - T_{i-1})}{h/2},$$
- from i cell side
$$P_i = \frac{k_iS(T_i - T)}{h/2},$$

where T – the current temperature at the border of the considered cells.

Based on the equality of heat flows, at the border of the cells $P_{i-1} = P_i$, we can find T – temperature on the border between them:

$$T = \frac{k_{i-1}T_{i-1} + k_iT_i}{k_{i-1} + k_i}.$$

Equating heat flows $P_{i-1} = P_i$, and we obtain the value of the effective thermal conductivity coefficient

$$k_{i-1,i} = \frac{2ki - 1k_i}{ki - 1 + k_i}. \tag{5}$$

So the change in energy $\triangle Q$ for i cells, based on (3), is determined by the relation

$$\triangle Q = \frac{\tau S}{h}(k_{i-1,i}(T_{i-1} - T_i) + k_{i,i+1}(T_{i+1} - T_i)). \quad (6)$$

The above approach for calculating the change in cell energy can be extended to the case of two-dimensional and three-dimensional problems in Cartesian coordinates.

2.2. Three-dimensional cylindrical cellular automata thermodynamic model

A significant part of technical objects has a cylindrical shape, that allows using the property of axial symmetry to reduce the dimension of the model and reduce the amount of computation [44].

Let's consider the motion of heat flows for a group of cells with a Neumann neighbourhood in the presence of axial symmetry of the simulation object.

Fig. 3 schematically shows a cell in a cylindrical coordinate system. Before determining the change in cell energy, it is necessary to determine the areas of the lateral surfaces of the cell.

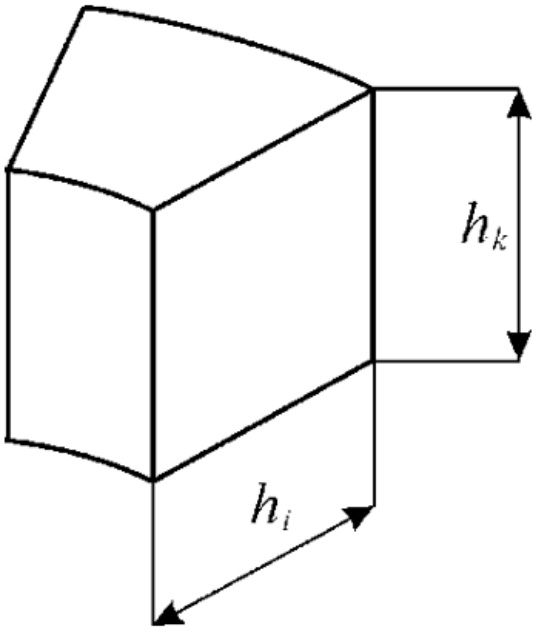

Figure 3: Three-dimensional image of a cell

Let's introduce the notation:
i – cell number in the radial direction, $i = \overline{1...i_n}$;
j – sectoral cell number, $j = \overline{1...j_n}$;
k – cell number along the axis of symmetry, $k = \overline{1...k_n}$;
h_i – radial cell length;

h_j – the sectoral width of the cell depends on the position of the cell in the radial direction;
h_k – cell height along the axis of symmetry;
n_i – number of cells in the radial direction;
n_j – sectoral number of cells;
n_k – number of cells along the axis of symmetry.

Fig. 4, 5, 6 show a schematic representation of a cell (i, j, k) and notations of its lateral sides.

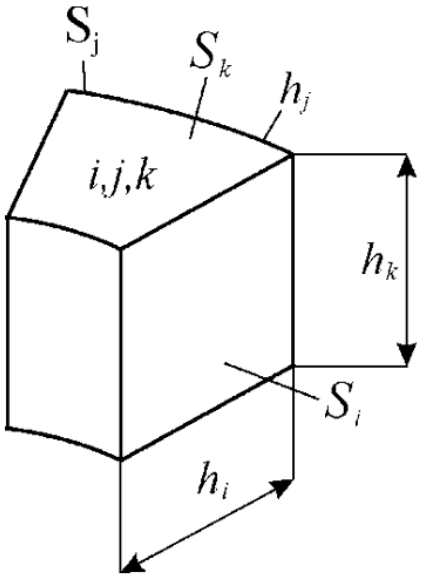

Figure 4: Schematic representation of a cell and notations of lateral sides

The sectoral width of the cell depends on the position of the cell in the radial direction, i.e. from i:

$$h_j(i) = \frac{2\pi h_i i}{n_j}.$$

The lateral sides of a cell are expressed in terms of the cell number, cell length and the number of cells along the axes:

$$S_i = h_i h_k,$$

$$S_j(i) = \frac{2\pi h_i i}{n_j} h_k,$$

$$S_k(i) = \frac{\pi h_i^2 (2i - 1)}{n_j}.$$

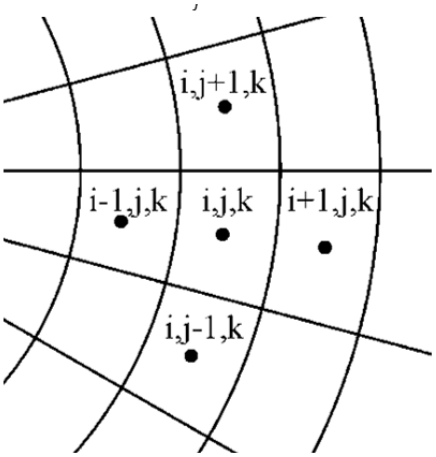

Figure 5: Schematic representation of cells in a cylindrical coordinate system (top view)

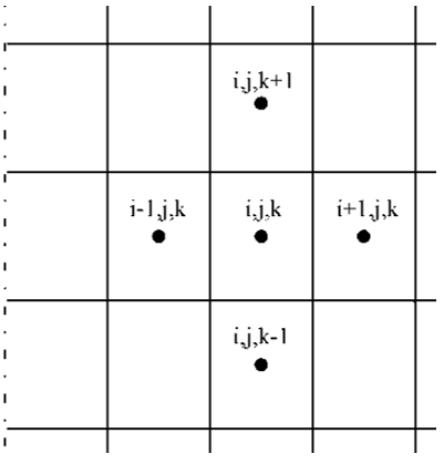

Figure 6: Schematic representation of cells in a cylindrical coordinate system (side view)

The change in cell energy for a cylindrical coordinate system consists of the sums of energy changes in the radial, sectoral directions and along the axis of symmetry of the body.

Thus, the change in energy for i, j, k–th cell

- in radial direction:

$$Q_{i-1,i}^{j,k} = \frac{k_{i-1,i}^{j,k} S_j(i) \left[T_{i-1} - T_i \right] \tau}{h_i},$$

$$Q_{i+1,i}^{j,k} = \frac{k_{i+1,i}^{j,k} S_j(i+1) \left[T_{i+1} - T_i \right] \tau}{h_i};$$

- in the sectoral direction:

$$Q_{j-1,j}^{i,k} = \frac{k_{j-1,j}^{i,k} S_j(i) \left[T_{j-1} - T_j \right] \tau}{h_j(i)},$$

$$Q_{j+1,j}^{i,k} = \frac{k_{j+1,j}^{i,k} S_j(i+1) \left[T_{i+1} - T_i \right] \tau}{h_j(i)};$$

- along the axis of symmetry:

$$Q_{k-1,k}^{i,j} = \frac{k_{k-1,k}^{i,j} S_k(i) \left[T_{k-1} - T_k \right] \tau}{h_k},$$

$$Q_{k+1,k}^{i,j} = \frac{k_{k+1,k}^{i,j} S_k(i+1) \left[T_{k+1} - T_k \right] \tau}{h_k}.$$

In the above formulas, superscripts indicate the same coordinates for neighbouring cells, and subscripts indicate the direction of the considered interaction.

A cell energy change is the sum of energy changes in all directions:

$$\sum Q_{i,j,k} = \tag{7}$$

In the above formulas, the unknown parameter is the effective thermal conductivity, that is calculated from the equality of heat flows between cells for a cylindrical coordinate system (Fig. 7).

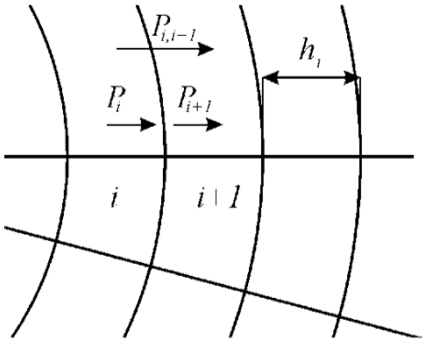

Figure 7: Heat flows between cells for radial heat distribution

Heat flow between cells i and $i + 1$ is determined by ratio

$$P_{i,i+1} = \frac{k_{i,i+1}(T_i - T_{i+1})}{h_i} \frac{2\pi h_i h_k i}{n_j}.$$

Heat flow to the border that separates cells:

- from i cell's side
$$P_i = \frac{k_i(T_i - T)}{h_i/2} \frac{2\pi h_i h_k (i - 0.25)}{n_j},$$
- from $i + 1$ cell's side
$$P_{i+1} = \frac{k_{i+1}(T - T_{i+1})}{h_i/2} \frac{2\pi h_i h_k (i - 0.25)}{n_j}.$$

Based on their equality of heat flows at the cell border $P_i = P_{i+1}$ we can find T – cell border temperature:

$$T = \frac{k_i T_i (i - 0.25) + k_{i+1} T_{i+1} (i + 0.25)}{k_i (i - 0.25) + k_{i+1} (i + 0.25)}. \tag{8}$$

Equate $P_{i,i+1} = P_i$ and we obtain the value of the effective coefficient of thermal conductivity for radial heat propagation

$$k_{i-1,i} = \frac{2k_i (i - 0.25) k_{i+1} (i + 0.25)}{i(k_i (i - 0.25) + k_{i+1} (i + 0.25))}. \tag{9}$$

When calculating the change in energy along the axis of symmetry and along the circumference, the effective coefficient of thermal conductivity is calculated similarly to the one-dimensional case using the formula (5).

3. Conclusions

The presented mathematical model can be integrated into an automated production control system, the components of which communicate in order to optimise the parameters of the production cycle.

We have given a description of a cellular-automaton thermodynamic model of solidification, taking into account the phase transition for the Cartesian and cylindrical coordinate systems, which differs from the existing ones by correctly considering the thermodynamic features of the solidification process.

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