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Modeling of impurities segregation phenomenon in the melt crystallization process by the continuous cellular automata technique

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ABSTRACT

This paper is dedicated to the problem of constructing a cellular automata model of the process of directed crystallization of binary solutions. The occurring processes of redistribution of impurities and concentration overcooling are emphasized. Previously known idea of the mechanism of overcooling action concentration is discussed in the description. The results of calculation of impurity concentration distribution along the sample fragment during crystallization are presented. Dependence of the temperature of the melting phase transition on the value of the impurity concentration is determined basing on the calculated impurity distribution. Graphic examples of the varieties of uneven impurity distribution as a result of overcooling concentration of the melt are given.

1. Introduction

It is well known that many physical properties of crystalline materials obtained by the method of directed crystallization are determined by the distribution of impurity in the melt and its ability to accumulate in the form of separate grains, cells etc. This occurs due to concentrated overcooling and leads to deterioration of the mechanical, electrical and physical properties of the material. It is one of the reasons for their fragility. A series of experiments is needed to investigate the optimal conditions for the growth of semiconductor materials with required properties. The time required is not always available, and the labor and material resources cost is rather high. Therefore, in recent years great attention is paid to the development of the technology of process simulation.

Spatial segregation is a complex process to be described in terms of mathematical equations. The imitation or agent-based models where certain rules of conduction can be assigned to each agent are the most popular and flexible techniques at present. One of such approaches is the cellular automata simulation technique. It not only provides a description of the physical properties of the material but can also predict changes on the micro-level.

The main difference of cellular automata from ordinary differential equation (DE) lies in the local rules by which the dynamics of the system is described. When using DE we assume the existence of some rules of averaged values over the whole system changes. In the case of the existence of such spacecraft the macro rules are optional. When using the CA the existence of such macro rules is also optional. It is enough to know the laws of the system's development on the microlevel in small spatial regions that make up the macrosystem.

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Another difference is discreteness of variables. For CA models there always exists a minimal discrete step, while for the numerical solution of DE this step can be reduced to infinitesimal values.

The combination of CA properties, such as the locality of conducting rules and the discreteness of variables, allows taking into account the fluctuations in the system without any additional assumptions.

So the main features of a complex dynamic system can be described by simple rules of management, defined from the behavior of the system over time.

CA are the most effectively used to describe the behavior of a system the collective behavior of which is determined by the local behavior of its constituent elements, when the system is highly heterogeneous, and averaging of variables throughout the system can hardly reflect its status adequately as a whole. Therefore, while modeling the melting process, accompanied by the first order phase transition, we chose the cellular automata technique.

Cellular automata were invented by von Neumann [1]; this proved the existence of a self-reproducing universal computer.

Then the idea became popular and many researchers are working on its development. So, several quality classes of cellular automata (CA) behavior, based on various statistical measures are defined in [2]. It was investigated how the cellular automaton is changed by varying entries in its rule table. These abrupt changes have either the character of bifurcations in smooth dynamical systems or that of phase transitions in statistical mechanical systems. Cellular automata classification is difficult. Wolfram classification scheme was developed, consisting of four quality classes, for which all cellular automata can be divided according to the type of evolution – homogeneous fixed point (class I), periodic (class II), chaotic (class III), and complex (class IV) ones [3]. He suggests reliable arguments that the achievements in the field of cellular automata are not isolated but very stable and are of great importance for all areas of science. Such definitions are mostly qualitative and can be interpreted in different ways. In [2] six classes of conduct which specify the classes of Wolfram's classification were listed. Other approaches to CA rules classification were detailed in the works by Chatee and Manneville [4], Gutowitz [5], McIntosh [6].

However, the classification alone is not enough. It is necessary to gain deeper understanding of the nature of the cellular automata interaction rules.

Despite a long period of research of cellular automata, the general theory of cellular automata has not yet been formed. But at the same time, the cellular automata are very successfully used to model various dynamic systems characterized by close interaction between the constituent elements, and this direction proves to be very promising. In recent years, the alternative approaches to numerical methods for problems of heat conductivity and diffusion are widely used. Cellular automata algorithms are quite successfully used [7,8] for this purpose. It should be noted that discrete models are used in most cases for calculation of diffusion processes [9], while the continuous models of cellular automata [10,11] are used to approximate heat transfer processes. In [12] Benito and Hernández prove that cellular automata technique is a suitable tool for modeling multi-interactive procedures. Specifically, they used arguments to confirm the simulation results obtained for the classical model of segregation Schelling [13].

Janssens [14] should also be mentioned here in regards to the subject of phase formation modeling using cellular automata. It shows the results of simulation of grain boundary motion when driven by the minimization of volume-stored energy as well as when it is curvature-driven. It also gives an example of a hybrid model that combines cellular automata with the description of diffusion computing and dissolving of precipitation under abnormal grain growth. Furthermore, Golab et al. [15] should be taken into consideration where calculations of austenite–ferrite phase transformation in steels are performed using cellular automata model. Researchers describe the rules of transition for the initial and subsequent growth taking into account internal variables for each CA cell. A qualitative model of the phase transition within the developed cellular automata was presented and sensitivity analysis of the developed complex microscale austenite to ferrite phase transformation model was performed. The possibility of describing complex phenomena and processes using cellular automata enables to simulate not only the phase transition during the crystallization process, but also to sophisticate such a model by the presence of emerging concentration overcooling, which is not modeled in previous works.

In this research we use the method of continuous cellular automata. As it was previously shown in [16], it is possible to display not only the qualitative, but also the quantitative aspect of the modeled process by calculating the time of a CA interaction. This makes it possible to determine the characteristics of the process at certain points of time. Due to its simplicity and versatility, this method is a good alternative to the previously known classical methods for solving problems of heat conductivity, diffusion of impurities, modeling of phase transitions. The description and results of application of continuous cellular automata method for modeling the directional crystallization of binary solutions in dynamics are presented in this paper. Here the segregation and dependence of the phase transition temperature on the material composition is taken into account, because under certain conditions it can lead to the phenomenon of concentration overcooling and, accordingly, to uneven geometry of the crystallization front.

2. Preliminaries

It is known that solubility of impurity components in the liquid phase and equilibrium solid phase of the basic substance are different. This is due to different values of the chemical potentials of impurities in the solid and liquid phases.

The difference between the ratio of components in liquid and its equilibrium solid phase is characterized by the distribution coefficient [17]:

$$K_0 = C_S/C_L, \tag{1}$$