1. Introduction

A large number of technologies that define modern production, associated with multi-factor processes of crystallization, create prerequisites for their comprehensive review in a multidimensional space [1–3].

The transition to practical solution of this task is greatly facilitated by the visualization of these processes [4]. One can make a cautious assumption that the accumulation of relevant multidimensional visualization techniques will enable creation of program systems that may solve a wide range of tasks of the formation of crystals, similar to MATLAB software, which successfully solve the tasks of computational mathematics [5].

The desire to find out the special role of time in the development of diverse conditions and phenomena related to crystallization, for example, in polymeric compositions in asphalt concretes, leads to a number of assumptions that deserve serious attention. Defending the view of reality and objectivity of time, G. J. Whitrow notes that “the central point of discussion is the status of “formation” or happening as well as the past, present and future; in other words, those features of time, for which there are no spatial analogies” [6]. In this regard, the spatial modelling of crystallization processes with the inclusion of the parameter of time, as the fourth dimension, is quite an actual task.

2. Analysis of scientific literature data and the problem statement

The modelling of the processes of crystallization is due to the complexity of implementing an optimal automatic control of the process itself, which, apparently, will become an integral feature of any production in the not too distant future.

A rather active research is going on in this direction. For example, a device was designed for measurement of distribution of multivariate sizes of particles in the process of crystallization, which allows their selection from the stream through the cell of a particle to obtain their images in the form of suspension out of two perpendicular directions [7].

The researchers [8], aware of achievable scope of particle sizes and possible alternatives to the process of continuous crystallization, determine the sizes of the particles, defined by the configuration of the process. The influence of uncertainty of kinetic parameters required to define them is also taken into account.

There is experience in designing and managing various operations of crystallization that contributes to the development of systems of control and management of technological processes. The system in the software is implemented that allows the user to create and validate various situations through systematic automated frame [9].
The enhanced capacities of managing the process of crystallization can be illustrated by the studies associated with the control of parameter of viscosity. This is achieved by connecting differential scanning calorimeter and thermocouples to monitor the crystallization process, followed by building a diagram of temperature and time of conversion with allocation of crystal phases [10]. The conducted studies have shown the possibility of substantially increasing the qualitative characteristics of the tested material through the management of the process of crystallization.

The active use of kinetic analysis allows forecasting of information regarding the fragility of the studied materials, obtained in the process of crystallization under the conditions of kinetics of phase transformation and optimize energy costs [11], as well as it creates preconditions for increasing thermal stability of crystals [12]. It is being proved that a thorough kinetic analysis can lead to a reliable, accurate and detailed description of complex processes, as well as to interpreting any visible trend occurring in experimental data [13].

In the papers of which the authors are aware of, in the analysis of the problem of crystallization, either the questions of the process planning are discussed, or the questions of taking into account the factors of influence and control over the process. The process is not addressed holistically, in development in space and time by predetermined trajectory of optimal control of the process. The analysis of the thermodynamic function of Liapunov shows that pulsating, vibrational modes due to the actual process of crystallization must be sought during the crystallization of substances for which the processes of crystallization occur at great distance from equilibrium. In this connection, it should be noted that in order to study the stability of the process, Liapunov, as the original equation, adopts the equation

$$\frac{dy}{dt} = Y(t, y_1, y_2, ..., y_n)$$

to characterize the multifactor process evolving over time.

Addressing multidimensional space during crystallization is objectively determined. In particular, the studies of pulsed radio emission during the crystallization of water found that the crystallizing water was a system with strongly heterogeneous permeability. It was also found that the dielectric permeability, considered in a four-dimensional space and time of conversion should lead to a change in capacitive coupling with a probe and cause emission of electric signals [14].

Of interest here is the experience of visualization of the process of the crystallization of polymers in a three-dimensional space conducted in the National Scientific Centre of Kharkov Institute of Physics and Technology (Ukraine). In particular, the visualization that used the video recording allowed determining the growth rate of crystallized phase and the time of the closure of channels during the movement under pressure [15].

There are endless options of a combination of factors that determine the properties of materials during crystallization. The solution of the task of the optimization of crystallization process over time will significantly improve the accuracy of forecasting and implementing planned properties of materials and substances obtained in the process of crystallization, and manage this process.

3. The purpose and objectives of the study

The aim of the study is the visualization of the modelling of crystallization process, allowing presenting vividly the results of the analysis in a three-dimensional space and time, which contributes to a better understanding of the processes, as well as evaluating and finding optimal control of the process of crystallization.

To achieve the set goal, the following tasks were defined:
- to perform theoretical justification of the possibility of the visualization of the process of crystallization in a 4D space;
- to develop the concept of the modelling of the visualization of the process of crystallization in a 3D space;
- using as the example the free energy of the forming solid substance and the speed of particles (atoms, molecules), to show vividly in a 4D space that the parameters of the factors change during the change in the crystallization temperature under the influence of actual conditions in time.

4. Theoretical aspects of the visualization of processes in space and time

Space-time (s.-t.) is a geometric design that describes the spatial and temporal relations in physical theories in which these relationships are treated as mutually dependent. The development of the basic provisions of the s.-t. relates to the formulation and systematization of the major provisions of the theory of relativity. S.-t. in this theory is a four-dimensional pseudo Euclid space with a linear element

$$ds^2 = c^2 dt^2 - dx^2 - dy^2 - dz^2,$$

where x, y, z are spatial coordinates, and t is a temporal coordinate, c is the speed of light. This coordinate system is called the Galilean in physics and it corresponds to the inertial reference system (i. r. s.) [16]. (In the special theory of relativity, i. r. s. is usually set by the Galilean coordinate system, in classical mechanics – by the Cartesian coordinate system.) In the studies by Galilei, the ability of Galilean transformation deserves attention, which maintains the spatial dimensions of bodies and the durations of physical processes [17]. The transition between different Galilean coordinate systems, with appropriate i. r. s. moving relative to each other, occurs with the help of the Lorentz transformation [18]. This transformation allows the spatial reflection of a set of points in time, which from the standpoint of physics is a transformation of transition from one inertial reference system to another, moving with the speed V relative to the first one.

Given that the Lorentz transformation is analogous to orthogonal transformations (or generalization of the notion of movement) in Euclidean space, it is possible to associate in Minkowski universe [19] two Galilean coordinate systems Fig. 1.

Also taking into consideration that the Galilean coordinate system differs from the Cartesian coordinate system only in applications of reference system [17], one can accept, with a sufficient degree of substantiation, the given method of the visualization of a four-dimensional space as a first approximation.

It should also be noted the comment by A. Einstein that “the relativity theory has been often criticized for unduly
attributing the central theoretical role to the phenomenon of propagation of light, basing the notion of time on its laws. The situation, however, is more or less like this. To give the notion of time the physical sense, there must be some processes, which would make it possible to establish a link between the various points in space. The question of what kind of processes are selected with such a definition of time is irrelevant. For the theory it is convenient, of course, to select only those processes about which we know something definite. The propagation of light in the vacuum, due to the researches of Maxwell and Lorentz, fits this purpose much better than any other process, which could be considered [20].

From here one can make an important conclusion. In the system \( c = \text{the speed of light in a vacuum is constant.} \) To solve an applied task, it can be replaced by the constant, which satisfies best the requirements of the process being analyzed. A. Einstein arrived at a conclusion that the principle of relativity was universal. Based on the postulate that “all the laws of nature are the same in all inertial systems of reference”, he found out that not only mechanical, but also all the physical laws were the same in all inertial systems of reference [21]. For example, one can accept the maximum possible set (or calculated) hardness, transparency, crystallization temperature, the speed of crystallization and other control parameters of the process with the specified characteristics.

Therefore, the managed processes, considered in a 4D space, can be the object of applied analysis with the help of the theory of s–t. It is necessary to note that the available results of the research of the processes in a four-dimensional space relate mainly to mathematical dependencies. As a rule, the complex functions and functions with three variables, in a 4D space, are explored, using interactive medium, for example, [22] and others.

However, this experience has somewhat abstract character without reference to any technical, industrial or technological processes.

The BIM (Building Information Modelling) system is also known as a building information modelling. Nevertheless, the multidimensionality in this system is limited to coloring the parts or nodes, on the axonometric representation on the plane, which characterizes the sequence of implementation of the phases of the work over time [23].

5. Formulation of the concept of the modelling of the visualization of the process of crystallization in a 3D space

The first task is to offer a theoretical framework to analyze the spatial distribution, study of the likely situations and forecast of results. As a form of analysis of crystallization, we suggest using the function, for example, of the type:

\[
Y = f(X_1, X_2),
\]

where \( Y \) is, for example, temperature; \( x_i = 1, \ldots, n \) are technological, physical, chemical, etc. factors that depend on \( Y \).

For example, \( x_1 \) is the free energy of a forming solid substance; \( x_{2, \ldots, n} \) is the speed of the movement of particles (atoms, molecules) relative to their average positions.

Let us consider a three-factor graphic model of crystallization in Fig. 2. The convex shape of the surface (2), selected as an example, is the easiest for illustration and understanding due to the possibility of its visualization in a 3D space. Curves – 1Y and 2Y connect the points with the same numeric values that characterize the temperature. Their projections – \( 1Y_c, 2Y_c \), \( 1Y_n, 2Y_n \) – are isotherms.

Let us consider the process of the beginning of crystallization of a supersaturated solution from point \( A \). As it is known, during the cooling of a supersaturated solution, electrical forces of attraction combine atoms or molecules in a crystalline solid substance. The formation of clusters of molecules (atoms) of crystallized substances (crystallizant) occurs first. The clusters form and break up with comparable frequency. They are present in a saturated solution (vapor) as well, but during the transfer of solution into an oversaturated state, their concentration increases. In the oversaturated medium, the clusters grow as a result of joining with the molecules of crystallizant, alternating with their separation from clusters. Primary aggregates, in turn, can combine into secondary aggregates, which are able to continue to grow by the way of attaching molecules, primary aggregates and nanocrystals. The formation of particles of each type occurs because of pair collisions of particles, followed by the subsequent ordering of aggregates of the emerged substance at any time [24].

As Fig. 2 shows, point \( A \) is located on isotherm \( 2Y_c \), characterized by, for example, the equilibrium temperature \( T_{ib} \), where the free energies of the liquid and solid states of a substance are equal and, to develop the process of crystallization, it is necessary to create the conditions under which the free energy of solid state is lower than the free energy of the liquid state. This is possible only when cooling below critical temperature – \( T_{cr} \). For example, in our model it is on the isotherm \( 1Y_c \), at which the spontaneous crystallization process begins in a substance.

The process of crystallization on \( 1Y \) may start in a particular system by the implementation of an infinite set of combinations of factors. For example, points \( B \) and \( D \), are showing some variants of achieving the crystallization temperature \( T_{cr} \) on level \( 1Y \).

Let us consider two variants of change from \( 2Y \) to the level of \( 1Y \), provided by the implementation of the process of crystal formation. Let us consider the vectors \( \overrightarrow{AB} \) and \( \overrightarrow{AD} \). Particular combination of factors corresponds to each of them: \( A \overrightarrow{x}_A, A \overrightarrow{x}_B, B \overrightarrow{x}_A, B \overrightarrow{x}_B, D \overrightarrow{x}_A, D \overrightarrow{x}_B \). From mathematical positions we assume the optimal option to be \( \overrightarrow{AB} \) because \( \overrightarrow{AB} \perp 1Y \) (to the tangent at point \( B \)), and it is the shortest distance between \( 2Y \) and \( 1Y \). It is known that the crystallization of each substance is characterized by individual, specific only to it, particular combination of factors [1]. Thus, the modelling of the process in which the shortest distance between isotherms is accepted as the criterion of optimality can be considered as ideal variant for a real substance.
The transition from A to B is characterized by a change in the free energy of substance – $0Bx_1$. Fig. 2 shows that $0Bx_2<0Ax_2$, therefore, during the transfer from level 2Y to 1Y, the free energy of a substance decreases which creates prerequisites for the development of the process of crystallization. Let us analyze the change in the speed of the movement of particles (atoms, molecules) relative to their average positions in the transition from level 2Y to 1Y. Given that $0Bx_2<0Ax_2$, i.e., the decrease in temperature is accompanied by a decrease in the speed of movement of particles relative to their average positions, therefore, the crystallization process evolves.

We similarly consider the analysis of the development of the process in point D. Fig. 2 shows that $0Dx_2<0Ax_2$, which points to a decrease in the speed of the movement of particles and to a possibility of development of the process of crystallization. However, $0Dx_2<0Ax_1$, therefore, the reduction of the free energy of a substance did not occur. Probably, the decrease of the free energy should be considered as a factor impeding the development of the process of crystallization. This can be explained, for example, by changes in the temperature, pressure, gravity force, chemical composition, concentration and dynamics of the medium, etc.

To compensate for the growth of the free energy of a substance, it is necessary to control the impact.

6. The model of crystallization in a 4D space

According to Minkowski, the position of an event is set by four coordinates – 3 spatial ones and one temporal [19]. Commonly used coordinates are $x_1=x$, $x_2=y$, $x_3=z$ where $x$, $y$, $z$ are rectangular Cartesian coordinates of an event in certain IRS and $x^\prime=ct$, where $t$ is the time of the event, $c$ is the speed of light in a vacuum. Geometric properties of a four-dimensional space are defined by the expression for the square of the distance between two events (interval) $s^2$:

$$s^2 = (dx^2 - dy^2 - dz^2), \quad (3)$$

where $dx^2$, $dy^2$, $dz^2$, are the differences in the coordinates of events, while $dt$ is the difference in their moments of time. The space with such $s^2$ is pseudo Euclidian.

To solve the task of the modelling of the process of crystallization in a generalized four-dimensional space, the expression (3) can be represented as:

$$s^2 = (dx^2 - dy^2 - dz^2), \quad (4)$$

where $x_1$ is the free energy of a solid substance; $x_2$ is the speed of the movement of particles (atoms, molecules) relative to their average positions; $y$ is the temperature. Then $x^\prime = I_1 t$, where $I_1$ is the speed of crystallization under ideal conditions, $I_2$ is the speed of crystallization under real conditions, $t$ is the time.

When moving from one inertial system of reference to another, the spatial coordinates and time are converted through each other by the quasi Lorentz transformation. It is known that the system of reference is called inertial if, in relation to it, any material point, free from interactions with other objects (isolated), is moving uniformly and in a straight line. In the special theory of relativity, Lorentz transformation is applied to the coordinates $(x, y, z, t)$ of each event when moving from one i.r.s. to another. The coordinates of any fourth vector are converted similarly [18].

The Lorentz transformations are transformations that keep the Minkowski metric intact. This means that the latter maintains the simplest type in them when moving from one inertial system of reference to another. The Lorentz transformations are equivalent to Minkowski metric’s orthogonal transformations in transition from one orthogonal basis (the basis, consisting of pairs of orthogonal vectors) to another or generalization of the notion of motion in Euclidean space. The total group of transformation consists of combinations of spatial representations in time and transformations that, from a physical point of view, are the transformations of the transfer from one inertial system of reference to another [17]. The transformations in the plane with a pseudo-Euclidean metric are a particular feature of the transformation, which is extremely important for our studies.

The transformations in the process of crystallization occur at collinear spatial coordinate system axes, if the inertial system of reference moves relative to the inertial system of reference $K$ at a constant speed (Fig. 1). In our task, by the speed we understand $I_1$ as conditional ideal crystallization speed; $I_2$ – actual speed of crystallization. The origins of the coordinates coincide in the initial moment of time in both systems [18]. Then the direct quasi Lorentz transformations for solving the task in a three-dimensional space and time will have the form:

$$x_i' = \frac{x_i t}{\sqrt{1-lo^2}}, \quad y' = y, \quad t' = \frac{t}{\sqrt{1-lo^2}}. \quad (5)$$

Obtained expressions allow moving on to the visualization of the process of crystallization in Minkowski universe.
7. Approbation of the model in a 4D space

Let us consider the graphic model (Fig. 2) of a two-factor function (2) in a three-dimensional space. Let us assume that all the set of possible combinations of factors, formalized by the surface \( Y = f(x_1, x_2) \) moves in time, where the world lines of material objects go to, forming certain hypersurface. Let us consider the simplest example, where the transition from level 2Y to level 1Y is characterized, for example, by vector \( \overrightarrow{AB} \), which, moving conditionally, creates plane \( \overrightarrow{ABA'B'} \). The plane reflects the process of crystallization in time (Fig. 3).

For the ease of explanation, we assume relative stability of the parameters of function \( Y = f(x_1, x_2) \) in time [25]. The conditions undergo the changes that characterize, for example, the cooling intensity, degree of saturation by a solid phase, content of impurities and numerous perturbations in the conditions of crystallization. The task is to show how crystallization occurs under real conditions, evolving over time.

Let us consider two particular variants of the model. We will consider movement of vector \( \overrightarrow{AB} \) in time within the specified parameters. Transformations at collinear spatial axes occur when moving with specific speed \( V \) while the origins of the coordinates coincide in the initial moment of time in both systems. As a result of the movement without spatial rotations in the specified system by object \( Y = f(x_1, x_2) \), the hypersurface and plane \( \overrightarrow{ABA'B'} \) are created. Then the length of segment \( \overrightarrow{AB} \) that characterizes the projection of the vector in time will be equal to the length of the vector, which characterizes its optimal position \( \overrightarrow{AB} \) in accordance with the adopted criterion of optimality.

Let us slightly change the ideal model. It is known that due to the influence of various external and internal reasons under real conditions, the deviations in the factors and conditions that influence crystallization are accepted. Then, for example, vector \( \overrightarrow{CD} \), under the influence of these causes, will gain the deviation, and while moving in space over time it is converted into vector \( \overrightarrow{C'D'} \). The parameters of vector \( \overrightarrow{CD} \), based on the above-mentioned criterion of optimality, will be distorted and its view can be represented as, for example, \( \overrightarrow{C'D'} \). The position \( \overrightarrow{C'D'} \) is not perpendicular to 1Y and, therefore, \( \overrightarrow{CD} \neq \overrightarrow{C'D'} \) and the position \( \overrightarrow{C'D'} \) does not match the adopted criterion of optimality. The influence of various factors such as the intensity of cooling, the degree of saturation by the solid phase, the content of impurities and perturbations in the conditions of crystallization may be suggested.

We develop further the concept of real conditions, for example, Fig. 4. The process begins at point A. The actual development of the process of crystallization is completed with the passage of time from A to \( B' \). Depending on the processes related to the crystallization that develop over time, in accordance with the Le Chatelier-Broun principle, vector \( \overrightarrow{AB} \) describes a rather complex path (Fig. 4). Due to the set of influence of factors and conditions, changing over time, the delay in reaction of the system of self-organization of substance to the changes in the process of crystallization, reorganization [26], and other reasons, the trajectory of the vector’s movement in time can be presented, in general, as a row of successive curves. The substance during crystallization, being in the state of sustainable chemical equilibrium, strives to return to the state of equilibrium under the external force, compensating for the received impact.

![Fig. 3. The model of s.-t., which illustrates the time points of Minkowski universe during the crystallization for the vectors \( \overrightarrow{AB} \) and transformations of \( \overrightarrow{AB} \) into \( \overrightarrow{A'B'} \) and \( \overrightarrow{CD} \) into \( \overrightarrow{C'D'} \).](image-url)
The confirmation of this hypothesis is the research results [27]. In particular, drawing on the large set of the results of spectral studies and the theory of nonlinear interaction of waves, the authors note that the analyzed processes represent real nonlinear resonant interactions of oscillating modes with the generation of higher vibrational states. They come close to electron states and effectively interact with them. Strong electronic oscillatory interactions lead to a change in the electron states and chemical bonds, which is the key to processes of melting and crystallization, displaying, according to the authors, a mechanism of self-organization of a substance [27].

For example, the crystallization is developing in the direction of vector $\overrightarrow{AB}$. Under the influence of real conditions, the vector undergoes vibrations in time relative to the specified destination and relative to a fixed axis $\overrightarrow{AA'}$. The vibrations indicate permanent changes of factors $x_1$ and $x_2$. Fig. 4 shows that, for example, the system of self-organization has failed to fulfill the task of the crystallization associated with achieving $1Y$ in accordance with the adopted working criterion of optimality and $\overrightarrow{AB} \neq \overrightarrow{AB'} \overrightarrow{A'B'}$. Therefore, $0Bx_1 \geq 0Ax_1$ during the process of crystallization, the growth of the free energy of a substance occurred that could be considered as a factor impeding the development of the crystallization process (similar to $0Dx_1 \geq 0Ax_1$ Fig. 2). To reach the optimal crystallization mode, the causes must be determined and the introduction of control actions into the process is necessary.

It should be noted that a rather complex surface, formed by the movement of vector $\overrightarrow{AB}$ in time (Fig. 4), is also the quantitative characteristic of the process of crystallization. The surface area, formed by the movement of the vector in time $t$, characterizes the energy costs and the potential qualitative changes in crystal formation, as the speed of the crystallization of polymers varies very widely.

The maximum speed of the formation of crystallization embryos will be achieved at the temperature that corresponds to the optimum ratio between potential energy of intermolecular interactions $E_{pot}$ and the energy of thermal motion in polymer $kT$, (which is defined by the position of vector $\overrightarrow{AB}$ during its movement in space and time (Fig. 4). If $E_{pot} \gg kT$, then the energy of thermal motion is low to effectively influence the reordering of macromolecules and the $I_r$ speed is minimal. When the temperature increases, the speed $I_r$ will accelerate. If $E_{pot} \ll kT$, then the fast formed crystalline areas are unstable and they disintegrate under the influence of thermal motion and speed $I_r$ is minimal. When the temperature decreases, the $I_r$ speed will increase. Then the $I_r$ will be maximum in the area of $kT–E_{pot}$ [28].

Depending on which properties one needs to obtain in the polymer composition, by possessing a mathematical model of the development of the process of crystallization in time, there appears a possibility to control the process for obtaining the material with defined properties at optimal energy costs.

8. Conclusions

The research results justify the ability to visualize the process of crystallization in a 4D space. Theoretical justification is based on the replacement of a constant – the parameter of the speed of light in a geometric design – space-time of the theory of relativity, by the parameter that matches the analyzed process best. The model of visualization of the crystallization process in a 3D space was designed, which is a theoretical platform for the analysis of spatial distribution, validation of the likely situations and forecast of the results of crystallization during the changes of parameters of factors of the crystallization of a polymer composition.

![Fig. 4. The model, which illustrates the time points of Minkowski universe for the vector of crystallization $\overrightarrow{AB}$ (transformations $\overrightarrow{AB}$ into $\overrightarrow{A'B'}$) with the account of the reaction to the exposure to internal and external activities](image-url)
By the example of the free energy of the forming solid substance and the speed of the movement of particles (atoms, molecules), it was vividly shown in a 4D space that during the change in the crystallization temperature under the influence of real conditions in time, the changes in the parameters of the crystallization factors of polymer composition occur. It has been established that the vector of the crystallization direction in space, under the influence of real conditions, undergoes vibrations in time relative to the specified direction, and describes a complex surface, which is a quantitative characteristic of the process of crystallization. This creates the prerequisites for the control of the process of crystallization and for obtaining the material with defined properties at optimal energy costs.

References