THEORETICAL ASPECTS OF VISUALIZATION OF THE PROCESS OF CRYSTALLIZATION OF THE BINDERING ORGANIC IN MINKOVSKY SPACE

VITALY S. BOROVIK,
VITALY V. BOROVIK,
DMITRY SKOROBOGATCHENKO
Volgograd State Technical University
Volgograd, Russian Federation
borovikv@mail.ru
borovikvv70@mail.ru
skor2004@rambler.ru

Abstract: *it achieved a visual representation of information about the crystallization process in the multidimensional space, which creates prerequisites for the development of software systems to solve a wide class of problems road construction. With the geometric interpretation Minkowski space-time, quasi-Lorentz and Einstein's concept concerning the concept of giving time physical sense, simulated the process of formation of crystals in the four-dimensional space. The 4D model space combines the physical three-dimensional space of the factors affecting the formation of crystals, and time. Visualization of the crystallization process in spacetime plays an important role, as having great cognitive and probative value, and contributes to a better understanding of crystallization processes, creates conditions to control the properties of materials in the process of crystallization.*

Keywords: *formation of crystals, multi-dimensional space, the Lorenz quasi-transformation; Minkowski space.*

Received: 20/09/2019 Accepted: 10/12/2019 Published online: 14/06/2020

I. INTRODUCTION

A large number of technologies that determine the modern road-building production associated with the use of bitumen modifiers, creates prerequisites for a comprehensive review of the process of crystallization of the binder in a multidimensional space [1-3]. Achieving improved material efficiency through enhanced functionality, as well as adaptability and facilitating the technologically automated mass production of the materials, at the stage of crystallization. The transition to the practical solution of crystallization task is greatly simplified by visualization of the processes developing in time [4]. You can make the conservative assumption that the accumulations of the corresponding multidimensional arsenal of imaging techniques allow to create software systems that solve a wide class of problems of crystal formation [5]. Charted fairly clear tendency to see the production processes in space and time, which creates prerequisites for more accurate forecasting calculations. According to US experts:

"The market for *3D* and *4D* technology, is expected to be worth US $ 127.84 billion in 2016 and will grow on average by 16.17 % between 2016 and 2022. The base year for analysis is taken in 2015, and the forecast period between 2016 and 2022. The market is segmented on the basis of technology, end-user industry, and geography" [6].

II. THE RELEVANCE, THE SCIENTIFIC SIGNIFICANCE OF THE ISSUE, SETTING GOALS AND OBJECTIVES

The desire to find a particular time in the development of diverse conditions and phenomena associated with the crystallization of materials, leading to a number of assumptions that deserve serious attention. Modeling of crystallization processes with the inclusion of the time parameter as the fourth dimension is a very urgent task. Modeling of crystallization process due to the complexity of the optimal process control, which, apparently, in the near future will be an integral feature of any production.

Appeal to the multidimensional space in the crystallization of objectively determined. In particular, when a pulsed radio studies on crystallization, such as water found that crystallizing water – a system with a strongly inhomogeneous permeability. It was also found that the dielectric constant, viewed in four-dimensional space ε (*x, y, z, t*), indicative of its temporal changes, which in the course of transformation must lead to a change in capacitive coupling with the probe and cause the appearance of electrical signals [7].

Active use of kinetic analysis allows predicting information about the fragility of the materials obtained in the process of crystallization kinetics of phase transformation conditions, optimizing energy costs [8], and also creates the preconditions for increasing the thermal stability of the crystals.

In the works of famous authors the analysis of crystallization problems addressed many questions about the process of planning or considering the factors of influence and control over the process, for example, [9,10]. The process is not considered comprehensive, the development in space and time on a predetermined trajectory of optimal process control.

It should be noted that both in domestic publications and foreign sources in visualization of the crystallization process in spacetime problem has not received a positive conclusion. Available results of the study process in four dimensions relate mainly to mathematical relationships, sophisticated features and functions of three variables in spacetime by means of an interactive environment, for example, [11]. However, this experience is somewhat theoretical without reference to how a technical, industrial, or technological process functions.

The objective of this study is modeling and visualization of the crystallization process, which allows visualizing the results of the analysis in three-dimensional space and time, contributing to a better understanding of the processes that will enter the evaluation and search for optimal process management.

II. THE THEORETICAL JUSTIFICATION FOR THE VISUALIZATION OF THE CRYSTALLIZATION PROCESS

The space – time (STSS) in special relativity theory (SRT) is a four-dimensional pseudo-Euclidean space with a linear element [12]

$$ds^2 = c^2dt^2 - dx^2 - dy^2 - dz^2 \quad (1)$$

Where *x*, *y*, *z* – the spatial coordinates, *t* – time coordinate *c* – the speed of light [13]. Fundamental importance is the remark of Einstein that "the theory of relativity is often criticized for the fact that it unfairly attributes a central theoretical role of the phenomenon of light propagation, establishing the concept of time in its laws. The situation, however, is approximately as follows. To give the concept of time, the physical sense, there must be some processes, which would give an opportunity to establish a connection between different points in space. *The question of what kind of processes are selected in such a definition of time is* ***irrelevant***. Beneficial to the theory, of course, choose only those processes for which we know something definite. The propagation of light in a vacuum thanks to the research of Maxwell and Lorentz for this purpose to a much greater extent than any other process which could be subject to review" [14] (Emphasis by the authors).

From this we can draw an important conclusion.

The system (1), from - the speed of light in vacuum - constant. Then, taking into account the remark of Einstein, for applications the speed of light can be replaced by a constant, which to the greatest extent meets the requirements of the analyzed process. Einstein came to the conclusion that the principle of relativity is the universal [15]. Consequently, as the constants can be set to take the maximum possible (or calculated) hardness, transparency, crystallization temperature, crystallization speed, and other process control parameters with desired characteristics.

III. VISUALIZATION OF THE SIMULATION CONCEPT

In the model as the original form of crystallization analysis it is proposed to use the function, for example, type:

$$Y = f\left(x_1, x_2\right) \quad (2)$$

Where *Y* – such as temperature; x_i , $i = \overline{1,n}$ – technological, physical, chemical, and other factors depending on the *Y*. For example, x_1 – the free energy of forming a solid; x_2 – speed of particles (atoms, molecules) about their average positions.

Consider Fig. 1 a three-dimensional graphical model of crystallization. Curves – 1*Y* and 2*Y* connect points with the same numerical values representing the temperature. Their projections – $1Y_1$, 2 Y_1, $1Y_2$, $2Y_2$, $1Y_3$, $2Y_3$ – isotherm. Consider the process of starting the crystallization of a supersaturated solution of point *A*. As can be seen, the point **A** is located on the isotherm characterized 2*Y*, for example, the equilibrium temperature T_0 at which the free energy of the

solid and liquid states of matter and are of the crystallization process is necessary to create conditions under which the free the energy of the solid state is less than the free energy of the liquid state. This is possible only when cooled below a critical temperature of – T_{cr} [16]. For example, in our model - the isotherm 1*Y*, in which a substance spontaneous crystallization process begins.

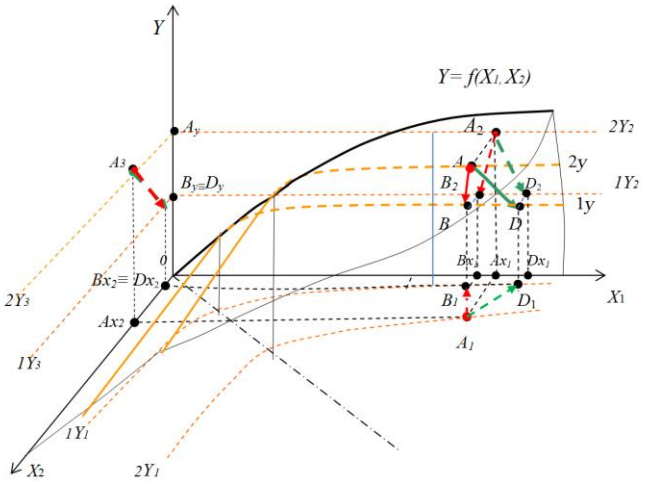

Fig. 1. *3D spatial model based on function (2), mapping the surface with different combinations of output at the crystallization temperature of the level 2Y (T_0) at 1Y (T_{cr})*

1*Y* crystallization process may begin in a particular system implementation by an infinite combination of many factors. For example, the points *B* and *D*, showing some embodiments output to achieve the crystallization temperature T_{cr} at 1*Y* level.

Consider two options to exit 1*Y* at the level 2*Y* provided by the implementation of the process of formation of the crystal. Consider the vectors **AB** and **CD**. Each of them corresponds to a combination of factors: Ax_1, Ax_2, Bx_1, Bx_2, Dx_1, and Dx_2. We will consider the best option **AB**, as **AB**⊥1*Y* (to the tangent at point *B*) and is the shortest distance between 2*Y* and 1*Y*. Going from *A* to *B* is characterized by a change in the free energy of the substance – $0Bx_1$. Fig. 1 that $0Bx_1<0Ax_1$ therefore, in the transition from 1*Y* to 2*Y* level comes free energy reduction substances than create the preconditions for the development of the crystallization process. We analyze the change in the velocity of particles (atoms, molecules) with respect to their mean positions in the transition from 1*Y* to 2*Y* level. Given that $0Bx_2<0Ax_2$ i.e. drop in temperature is accompanied by a reduction in the particle velocity relative to its middle position, therefore, the crystallization process is developed.

Similarly, we argue in the analysis of the development process in the point *D*. Fig. 1 shows that $0Dx_2<0Ax_2$, which indicates a decrease in the speed of the particles and the possibility of the development of the crystallization process. However $0Dx_1<0Ax_1$, consequently, decrease the free energy of substance happened, which can be considered as a factor hindering the development of the crystallization process.

IV. MATHEMATICAL MODEL

Minkowski status event is set four coordinates – three spatial and one temporal (1). The coordinates are usually used: $x_1 = x$, $x_2 = y$, $x_3 = z$, where x, y, z – cartesian coordinates of the events in an inertial reference system (ISO) and, $x° = ct$, where t – is time event, c – speed of light in a vacuum. Geometric properties of four-dimensional space defined by the expression for the square of the distance between two events (interval):

$$s^2 = \left(dx^o\right)^2 - dx^2 - dy^2 - dz^2, \tag{3}$$

Where dx^2, dy^2, dz^2 – the difference coordinate events and dt – the difference of their time instants. The space with s^2 – pseudo. To solve the problem of modeling the crystallization process in the generalized four-dimensional expression (3) can be represented as:

$$s^2 = \left(dx^o\right)^2 - dx_1^2 - dy_2^2 - dz^2, \tag{4}$$

Where x_1 – the free energy of the solid; x_2 – speed of particles (atoms, molecules) about their average positions; y – temperature. Then $x^o = I_i t$, where I_i – is the rate of crystallization under ideal conditions, I_r – crystallization rate under actual conditions, t – time. In the transition from one IRF to another spatial coordinates and time transform into each other by means of a quasi-Lorentz transformations. It is known that the inertial reference system is called, if in relation to it free from any interaction with other objects (isolated) material point moves uniformly in a straight line.

Transformations during crystallization carried out at a spatial coordinate axes collinear systems if ISO *K'* – ISO *K* moves at a relatively constant speed. Origins coincide at the initial time in both systems [17]. Then the lines quasi-Lorentz transformation to solve the problem in three-dimensional space and time will have the form:

$$\begin{aligned} x_1^{'} &= x_1 I_r t \Big/ \sqrt{1 - I_r / I_i}, \\ x_2^{'} &= x_2, \quad y^{'} = y, \\ t^{'} &= t - \left(\frac{I_r}{I_{ri}^2}\right) x_1 \Big/ \sqrt{1 - I_r^2 / I_i^2} \end{aligned} \tag{5}$$

V. PRACTICAL IMPLEMENTATION OF THE CONCEPT OF VISUALIZATION OF THE CRYSTALLIZATION PROCESS IN MINKOWSKI SPACE

For example, the entire set of possible combinations of factors that formalized the surface $Y = f(x_1, x_2)$ is moved in time, which are the world lines of material objects, forming some hypersurface (Fig. 2). Consider an ideal example when transition from 1*Y* 2*Y* level to level, is characterized, for example, the vector **AB**, which conventionally moving, forms a plane *ABA'B'*. As a result of moving c I_r certain speed without turning in a predetermined spatial object system $Y = f(x_1, x_2)$ plane and formed hypersurface. The *ABA'B'* length of the segment *A'B'*, which characterizes the projection of the vector in time, will be equal to the length of the

vector and is characterized by its optimum position **AB** in accordance with the criterion of optimality.

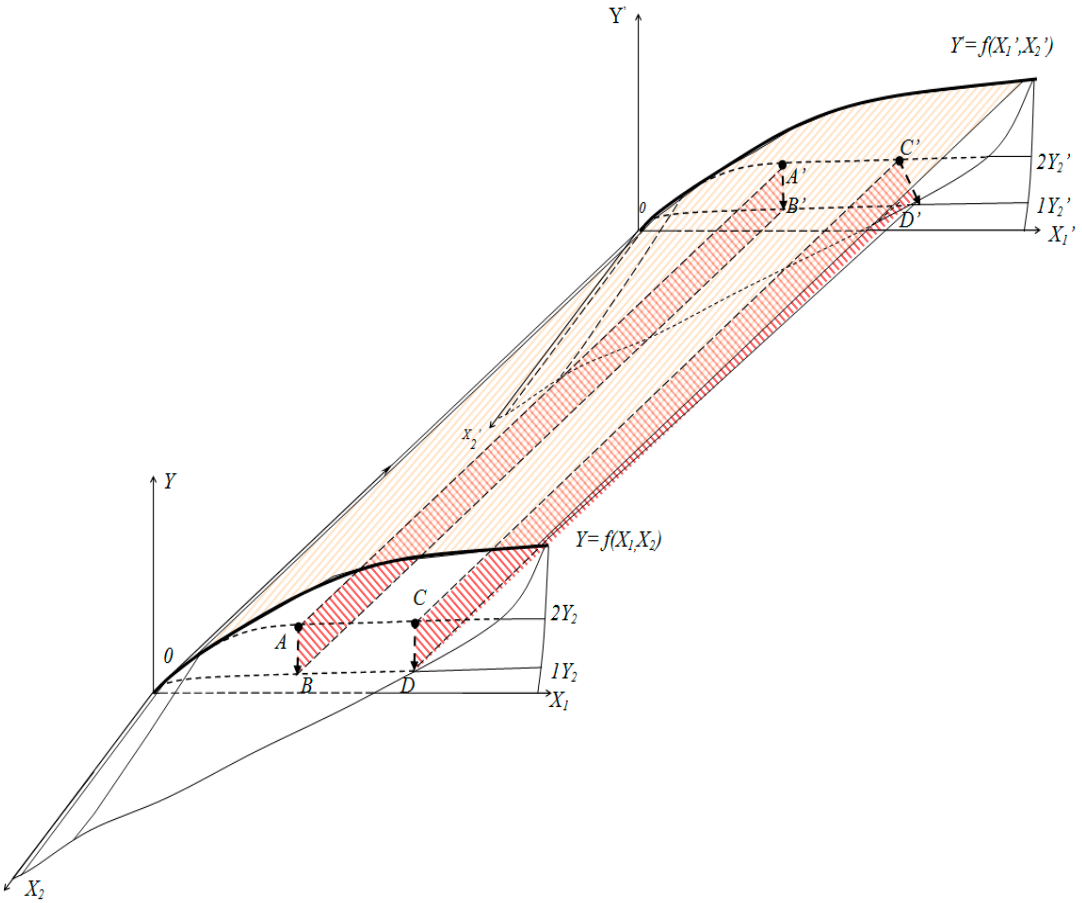

Fig. 2. *STSS Model illustrating the temporary section of Minkowski space in the crystallization of the vectors* ***AB*** *and* ***CD*** *(****AB*** *transformation in the* ***A'B'*** *and a* ***CD*** *in* ***C'D'****)*

The second option. Slight changes in the ideal model. It is known that due to the influence of various external and internal causes in the real world, permitted deviations in the factors and conditions that affect the crystallization. Then, for example, under the influence of vector **CD** receives these reasons deviation, and moving in the space over time, is converted into a vector **C'D'**. Settings vector **CD**, built on the above optimality criteria, and will get a distortion of his views may be presented, for example, **C'D'**. Position **C'D'** is not perpendicular to the $1Y'$ and, consequently, **CD≠C'D'**. This suggests the influence of various factors, such as cooling rate, degree of saturation of the solid phase containing impurities and crystallization conditions and disturbances etc.

Further develop the concept of the actual conditions, for example, Fig. 3. The process starts with the point *A*. The actual development of the crystallization process is completed with the

passage of time from *A* to *B'*. Depending on the processes associated with crystallization, developing in time, in accordance with the principle of Le Chatelier–Brown, the vector **AB** describes a rather complicated path (Fig. 3). By virtue of the cumulative impact of factors and conditions, time-varying delay in the reaction system of self-organization of matter [18] on the change in the process of crystallization and other reasons the path of the vector in time in general form can be represented, for example, a number of successive curves. The substance in the crystallization in a state of stable chemical equilibrium in external action seeks to return to equilibrium, compensating an impact.

Confirmations of this hypothesis are studies, for example, [11, and 12]. In particular, crystallization processes are accompanied by non-linear resonant vibrational modes of interaction with the generation of higher vibrational states. Strong vibration-electron interactions lead to a change in the electronic states and chemical bonding, which is a key for the melting and crystallization processes in what appears the mechanism of self-organization of matter.

For example, crystallization develops in the direction of the vector **AB**. Under the influence of the actual conditions vector oscillates in time with respect to a predetermined direction and relative to a fixed axis AA' . Fluctuations show permanent changes in x_1 and x_2 factors. Figure 3 shows that, for example, self-organizing system does not provide a solution to the problem of crystallization associated with access to 1*Y* in accordance with our criteria of optimality and **AB≠A'B'**. Consequently, $0Bx_1>0Ax_1$ during the crystallization process occurred the free energy of the substance growth, which can be considered as a factor hindering the development of the crystallization process (similar to $0Dx_1>0Ax_1$ Fig. 1). To reach the optimal mode is necessary to identify the causes and the introduction of control actions in the process.

The maximum nucleation rate of crystallization is at the temperature, which corresponds to the optimal ratio between the potential energy of intermolecular interactions *Epot* and the energy of thermal motion of the *kT*, (which is determined by the position of the vector **AB** while moving it in space and time (Fig. 3). If $E_{pot} >> kT$, then the energy of the thermal motion of small to effectively influence the repackaging of macromolecules and speed I_r. When the minimum temperatures will increase the rate of I_r. If $E_{pot} << kT$, then quickly formed crystalline regions are unstable and disintegrate under the influence of the thermal motion of the speed and I_r – is minimal. When the temperature drops I_r speed will increase. Then I_r will be maximum in $kT–E_{pot}$ [19].

Depending on what properties necessary to obtain a material having a mathematical model of the process of crystallization time is possible to control the process to produce a material with desired properties with optimum energy consumption.

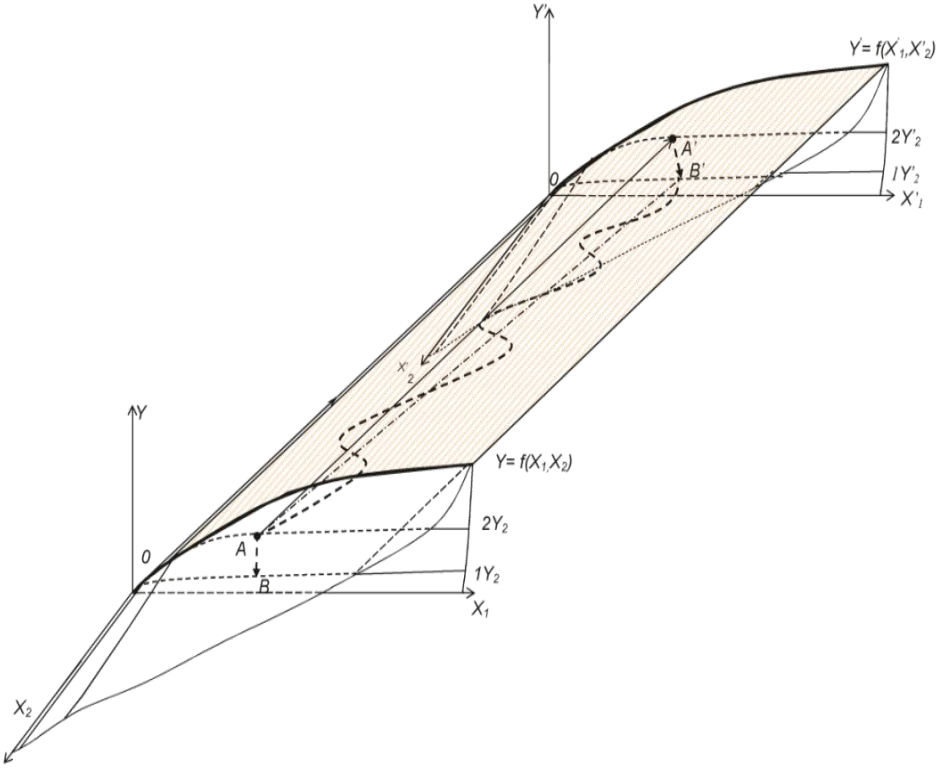

Fig. 3. *Model illustrating the temporary section of the Minkowski space for the crystallization of the vector* ***AB*** *(****AB*** *transformation in the* ***A'B'****), taking into account the response to the impact of external and internal influences*

VI. CONCLUSIONS

The possibility of visualization of the process of crystallization of polymer binder in the space Minkowski space is substantiated. The concept of visualization of the crystallization process in 3D space has been developed. The concept is a theoretical platform for analyzing spatial distribution and study of possible situations and predicts crystallization results when you change the parameters of factors. For example, the free energy of forming a solid and velocity of the particles (atoms, molecules), it is possible to demonstrate in spacetime, that when the crystallization temperature under the influence of the actual conditions of the time there is a change of parameters of crystallization factors. It is found that the crystallization of the vector direction in the space under the influence of channel real oscillates in time relative to the predetermined direction and describes a complex surface whose area is an integral characteristic of the crystallization process. Knowledge of quantitative characteristics creates conditions to manage the process and produce a material with specified properties at optimal energy consumption.

References

[1]. H. In. Bystrov. (2017) A new stage in the development of the regulatory framework for road asphalt // Science and technology in the road industry. 2017. No. 1. Pp. 2-6. 2.

[2]. A. S. Chernov, (2016) Modified asphalt binder with high resistance to aging /A. S. Chernov, A. V. Kalugin, I. V. Lazarev, Q. Zhao// Science and technology in the road sector. 2016. -No. 2. C. 11-12.
[3]. V.S.Borovik. Spatial and Time Simulation of the Traffic Safety Level Control Process / Borovik V.S, Borovik V.V., Lukin V.A. //Transportation Research Procedia.Volume 20, 2017, Pages 74–79 . Oxford, OX5 1GB, United Kingdom. (Scopus) DOI: 10.1016/j.trpro.2017.01.017
[4]. Yu.N.Maslovsky, S.V.Slipushenko, A.V.Tur, V.V.Yanovsky, "*3D* composite particles," in Functional materials, vol. 22, №1, 2015, pp. 69-78.
[5]. Igor I. Smolyaninov, Vera N. Smolyaninova. Experimental observation of melting of the effective Minkowski spacetime in cobalt -based ferofluids. arxiv.org/pdf/1504.04228v3. 2017.
[6]. *3D* & *4D* Technology Market by Technology - 2022 Markets and Markets By: marketsandmarkets.com Publishing Date: April 2016.
[7]. Y. Golovin, "Impulse radio emission in the crystallization of water," in Natural and Technical Sciences, Vol. 1, pp.158-160, 1996.
[8]. Yi-Hui Jiang, Feng Liu, Kai Huang, Shu-Hua Liang, "Applying Vogel-Fulcher-Tammann relationship in crystallization kinetics of amorphous alloys," in Thermochimica Acta, Vol. 607, pp. 9-18, May 2015.
[9]. S. Schorsch, T. Vetter, M. Mazzotti, "Measuring multidimensional particle size distributions during crystallization," in Chemical Engineering Science, Vol. 77, pp. 130-142, July 2012.
[10].T. Vetter, C. L. Burcham, M. F. Doherty, "Attainable Regions in Crystallization Processes: Their Construction and the Influence of Parameter Uncertainty," in Computer Aided Chemical Engineering, Vol. 34, pp. 465-470, 2014.
[11].Y. Sakai, "Four-dimensional Mathematical Data Visualization via Embodied Four-dimensional Space Display System," in Faculty 2 Research of Information Sciences and Arts, Toyo University, 2100 Kujirai, Kawagoe, Saitama, electronic resource.
[12].C. Moshe, "Group Theory and General Relativity, Representations of the Lorentz Group and Their Applications to the Gravitational Field," McGraw-Hill, New York, 1977.
[13]. Encyclopedia of Mathematics. Vol. 4. Publisher Soviet Encyclopedia. Moscow, 1984.
[14].A. Einstein, "The essence of the theory of relativity. Foreign Literature Publishing House," Moscow, 1955. pp. 28.
[15].A. Einstein, "The basic ideas and problems of the theory of relativity," in Collection of scientific works, vol. II. Moscow, 1966. pp. 120.
[16].Chemistry and Chemical Engineering. Crystallization rate theory process, electronic resource.
[17].Encyclopedia of Mathematics. Vol. 2. Publisher Soviet Encyclopedia. Moscow, 1984. p. 562.
[18].I.V. Melikhov, "Crystallization as the process of self-organization of matter," VIII International scientific conference "Kinetics and mechanism of crystallization. Crystallization as a form of self-organization of matter," Ivanovo, 24-27 June 2014.
[19].N.E. Kornienko, A.D. Rud, "Resonant vibrational self-organization of diamond-graphite states in Multidimensional carbon," VIII International scientific conference "Kinetics and mechanism of crystallization. Crystallization as a form of self-organization of matter," Ivanovo, 24-27 June 2014.