Computer 3D-simulation of the temperature and diffusion kinetics of SHS in the closest packing of Ni@Al “core-shell” mesocells for modes with variable values of the key ignition parameters

I A Shmakov¹ and V I Jordan¹²

¹ Department of Computing Techniques and Electronics, Altai State University, 61 Lenina ave., Barnaul, 656049, Russia
² Khristianovich Institute of Theoretical and Applied Mechanics, Siberian Branch of RAS, 4/1 Institutskaya str., Novosibirsk, 630090, Russia

E-mail: ihammers.sia@gmail.com, jordan@phys.asu.ru

Abstract. The paper presents the results of computer 3D-simulation of the temperature and diffusion kinetics of SHS in a test model cluster of Ni-Al particles for modes with variable values of the key parameters of the SHS combustion wave ignition. The key parameters for the SHS combustion wave ignition were chosen as follows: the initial temperature for preliminary heating of the Ni-Al particles mixture, the ignition temperature of the combustion wave in the mixture of Ni-Al particles, the duration of the action of the heat pulse until the combustion wave ignition, and the thickness of the ignited layer in the mixture of particles. A program has been created to generate a test model cluster in the form of the closest ball packing of the Ni@Al “core-shell” mesocells (CBP-structure cluster of the Ni@Al “core-shell” mesocells). Using such a CBP-structure cluster, was continued a testing of created software package intended for 3D-simulation of SHS macrokinetics in a heterogeneous particle mixture, taking into account parallel MPI-calculations. In addition, the value ranges of the key parameters of the SHS combustion wave ignition for which the simulation results are in adequate agreement with the experimental data are determined as the parameters of the program model for SHS-simulation. The results of computational experiments have shown that diffusion kinetics is interrelated with temperature kinetics, and in mesocells with different locations within the CBP-structure cluster, the formation of intermetallic phases occurs inhomogeneously.

1. Introduction

Modern mechanical engineering is showing great interest in the development of high-intensity technologies using scientific advances in the field of materials science. The creation of new materials with unique functional properties remains an urgent task in scientific research, both in theoretical and experimental terms. Among such effective technological methods for obtaining new materials, an important place is occupied by the process of “self-propagating high-temperature synthesis” (SHS), which occurs in a powder mixture of fine particles from various metals, ceramics and other components. The SHS process in a powder mixture is initiated by the action of a heat pulse, resulting in an intense exothermic reaction in the form of a propagating combustion wave along the mixture of particles due to heat transfer from layer to layer. The kinetics of SHS is influenced by various factors, incl. the packing structure of the reactant particles and the porosity of the mixture, as well as the ignition parameters of
the mixture (the initial temperature of the mixture heating and the ignition temperature of the mixture, the exposure time and the power of the heat pulse during the ignition of the mixture, the thickness of the initial layer when it ignites, etc.).

The search for modes in which the target products of the SHS reaction open up prospects for their use in modern industry is often quite costly in terms of time and cost. Therefore, computer simulation helps to significantly reduce the time spent searching for optimal control modes for the SHS process. Carrying out computational experiments at the simulation stage allows verification of the adequacy of the proposed physical and mathematical models of SHS. To simulate the generation of the structures of the packing of a mixture of particles, the previously developed program [1, 2] is used, which allows one to obtain a "pseudo-stochastic" distribution of particles in the spatial structure of the mixture with different particle sizes and different porosities of the powder mixture. For mixtures with a low level of porosity (30% or less), a special program for generating a test structure "closest ball packing (CBP)" was developed, in which flat layers are characterized by a square symmetry of the arrangement of spherical "mesocells" in the form balls (see figures 1 and 2). The space filling factor of the mixture volume in the form of such a CBP-structure cluster, which was used in [3] and in this paper, corresponds to approximately 70% (with a porosity of about 30%). The spatial structure of the mesocells included in the CBP-structure cluster is shown in figure 2(b, c) and for it we will use a conventional notation in the form Ni@Al "core-shell". That is, there is a large Ni particle in the core of the spherical mesocell, and Al particles in the shell.

The aim of this work is to refine the model concepts of the SHS initiation process and study the temperature and diffusion kinetics of the SH-synthesis of intermetallic compounds when the parameters of combustion wave ignition in the CBP-structure cluster of Ni@Al “core-shell” mesocells change.

2. Model representation of CBP-structure cluster of Ni@Al “core-shell” mesocells and description of variable key parameters of SHS combustion wave ignition

In this paper, we use model 3D-representations of the SHS process in the Ni-Al system based on the equations of heat conduction with the temperature-activation Arrhenius function and diffusion kinetics with the kinetic function of homogeneous kinetics for single-phase regions (Ni3Al, NiAl, etc.) [4, 5]. In [3], both the model representations of the equations of heat conduction and diffusion kinetics and the algorithmic foundations of their solution are presented in sufficient detail. Namely, to solve the heat equation, a software-implemented implicit scheme of two-cyclic splitting of the time layer into 7 intermediate time layers is used, which is based on the symmetric Crank-Nicholson scheme. To solve the problem of diffusion kinetics, Runge-Kutta grid schemes [3, 6, 7] are used to numerically solve the diffusion equations and balance relations at moving interphase boundaries in each mesocell (figure 2(c)) of the CBP-structure cluster, as a result of which, for each of mesocell, the radii \( r_j(t) \) of homogeneous phase interlayers varying in time are determined. The input data for the software package that implements the algorithmic foundations of the joint solution of the equations of heat conduction and diffusion kinetics is an external disk file that stores information about the CBP-structure cluster (figure 2 (a)). Let us consider in more detail the model representation of the CBP-structure cluster used for simulation of the SHS macrokinetics.

In authors paper [3], figure 1 shows examples of CBP-structures in which flat layers have a square symmetry of the arrangement of mesocells in them. In the fourth fragment of this figure (figure 1(d)), when displaying the simplest CBP-structure cluster in [3], some inaccuracies were made, therefore, in this paper, a similar figure with the necessary adjustments is shown again in full form (see figure 1). In the caption to figure 1, two parameters are indicated: M the number of flat layers with a square symmetry of the arrangement of mesocells in them; N is the number of mesocells located along each of the two directions X and Y in each flat layer of mesocells (for odd layers, the value of N is 1 more than for even ones).
Figure 1. 3D closest ball packings (CBPs): flat layers with square symmetry of mesocells arrangement (NxN) [3]: (a) M=9; NxN=5x5 – odd layer; NxN=4x4 – even layer; (b) M=3; NxN=3x3 – odd layer; NxN=2x2 – even layer; (c) M=3; NxN=2x2 – odd layer; NxN=1x1 – even layer; (d) a simplest CBP-structure cluster in the parallelepiped form was obtained using 6 flat sections passing through the centers of 8 cornered balls of CBP-structure show on the figure 1(c).

The sample of the test structure (figure 2(a)), which was used as the CBP-structure cluster in the process of the SHS macrokinetics simulation, is a parallelepiped that is more elongated in the direction of the Z-axis in relation to the structure shown in figure 1(d). The CBP-structure cluster in the upper part of its volume captures part of the volume of the central ball (mesocell) from the 4th layer of CBP-structure. The height of CBP-structure cluster is 170 µm, and the lower and upper bases of the cluster are 100x100 µm in size. The central whole ball (mesocell) in the CBP-structure cluster touches four lateral faces of the cluster (parallelepiped), since the diameter of the central mesocell in the 2nd layer, as well as the diameter of other balls (mesocells), is 100 µm. In the lower part of the cluster, in its corners, there are four lobes of 1/8 of one ball volume (the volume of the mesocell) each, and in the upper corners there are four lobes with volumes approximately equal to 1/5 of the ball volume (the volume of the mesocell). In addition, it should be noted that in the void regions adjacent to the mesocells of the even layers, there are 8 fine Al-particles in the form of cubic dense structures. In figure 2(a) such structures of 8 Al-particles are located under the central and above the central ball (they are not visible in figure 2 (a)).

Figure 2. Images of model structures: (a) the CBP-structure cluster using for 3D-computing simulation of SHS macrokinetics; (b) the spatial structure of the Ni@Al “core-shell” mesocell before the SHS process (T < 933 K); (c) the spatial structure of the Ni@Al “core-shell” mesocell in the SHS process (T > 933 K); the phases: ε — Ni$_3$Al, δ — NiAl, γ — Ni$_2$Al$_3$, β — NiAl$_3$.

In figure 2(b, c) show the spatial structures of a Ni@Al “core-shell” mesocell in the section, which was also given in [3]. In the center of the mesocell there is a spherical Ni-particle of radius $R_Ni = 30$ µm, and in its spherical shell 20 µm thick there are Al-particles of radius $R_Ai = 10$ µm, which are in a solid state (figure 2(b)) at a temperature lower than the melting temperature of Al (at T < 933 K). During SHS, the temperature of the combustion process turns out to be higher than the melting temperature (T > 933 K).
K), and Al-particles in the shell of the mesocell form a layer of liquid melt. In this case, homogeneous diffusion layers - spherical interlayers of intermetallic phases (intermetallic compounds), shown in figure 2 (c), are formed at the “core-shell” interface of the mesocell as a result of the SHS reaction. The time-varying radii \( r_i(t) \) of homogeneous phase interlayers are determined using numerical Runge-Kutta schemes, as mentioned above, as a result of solving the diffusion equations and balance ratios at movable interphase boundaries [3] in each mesocell of the CBP-structure cluster. In paper [3], “primary” testing of the created software package was carried out, intended for 3D-simulation of SHS macrokinetics.

In this paper, using the created software package, computational experiments were carried out, in which the values of the key parameters of the program model of the procedure for 3D-simulation of SHS macrokinetics were determined, which confirm a sufficiently high degree of adequacy of the simulation results to experimental data.

Based on the known reference data for the intermetallic phases of the Ni-Al binary system, for example [5], in the program model of the procedure for 3D-simulation of SHS macrokinetics were fixed the values of thermokinetic and diffusion parameters given below in the table 1 (\( \rho \) is the phase density; \( Q \) is the thermal effect of SHS reactions during the formation of intermetallic phases; \( D \) is diffusion constant for phases).

| Table 1. Thermokinetic and diffusion parameters of intermetallides. |
|------------------------|-----------------|-------------------------|
| \( \rho, \text{kg/m}^3 \) | \( Q \times 10^{-6}, \text{J/kg} \) | \( D \times 10^{-6}, \text{μm}^2/\text{s} \) |
| Ni3Al                 | 7200            | 0.7757731               | 10          |
| NiAl                  | 5900            | 1.374171                | 4.8         |
| Ni2Al                 | 4760            | 0.8619088               | 240         |
| NiAl3                 | 3900            | 0.8911564               | 600         |

As the variable parameters of the program model of the procedure for 3D-simulation of SHS macrokinetics, as already mentioned in the introduction to this paper, the following key parameters of the ignition of the SHS reaction were selected: 1) \( T_0 \) is the initial heating temperature of the entire particle mixture; 2) \( T_{ign} \) is the ignition temperature of the combustion wave in the initial flat layer of a particle mixture (the layer thickness is equal to \( H_{ign} \)); 3) \( t_{ign} \) is the time of action of a heat pulse upon ignition of a combustion wave in the initial plane layer of a particle mixture with the temperature \( T_{ign} \) being kept in it; 4) \( H_{ign} \) is the thickness of the initial flat layer in which the ignition of the SHS combustion wave is initiated by keeping the temperature \( T_{ign} \) within the time \( t_{ign} \). After the time \( t_{ign} \) has elapsed, the limitation on keeping the temperature \( T_{ign} \) in this layer is removed and the temperature in this layer (as well as in other layers of the mixture) is changed (controlled) in accordance with the laws of heat transfer (“free” boundary conditions begin to operate).

3. Results of the simulation computational experiments

In a series of computational experiments (more than 50) on simulation the temperature and diffusion macrokinetics of SHS, the values of the four key parameters of the combustion wave ignition varied with certain steps. Then, for each variant of the values of the four key parameters, a set of temperature profiles was calculated and visualized in order to analyze the temperature kinetics of SHS. Each temperature profile in such a set corresponds to a certain number of the time layer, in other words, the number of iterations over the corresponding index variable. In the legends to figures 3, 5 and 7, each individual graph of the temperature profile is associated with the number of iterations and, multiplying it by the time step of the grid calculations \( \tau = 10^{-8} \text{s} \), we obtain the current value of the moment in time corresponding to the profile. For example, the number of iterations 20000 corresponds to a time of 0.2 ms (or 200 μs).

In addition, for each variant of the values of the four key parameters, sets of time dependences of the relative radii of intermetallic phase interlayers were calculated and visualized both for cornered
mesocells (with 1/8 and 1/5 fractions) and for the central whole mesocell. The values of the relative radii of the spherical phase interlayers are determined by normalizing the absolute radii of the phase interlayers to the mesocell radius \( R_c = 50 \mu m \). The difference in the values of the relative radii of adjacent phase interlayers, equal to \( (r_i(t) - r_{i-1}(t))/R_s \), determines the relative thickness of the \( i \)-th phase interlayer. Changes in the values of the relative radii of the phase interlayers (or their thicknesses) with time allow one to analyze the diffusion kinetics of SHS (figures 4, 6 and 8), i.e. analyze in time the formation and decay of intermetallic phases within each mesocell. When performing grid calculations in computational experiments, the step along the spatial coordinates \( X, Y \) and \( Z \) was equal to 1 \( \mu m \) (in the software package, the parameter \( h = 1 \mu m \)).

In computational experiments, the initial temperature \( T_0 \) of heating a mixture of Ni-Al particles varied in the range from 600 to 1000 \( K \) with a step of 100 \( K \); the temperature \( T_{ign} \) of a combustion wave ignition in a particle mixture - from 1100 to 1600 \( K \) with a step of 100 \( K \); the time \( t_{ign} \) of the effect of the heat pulse until the moment of the combustion wave ignition in the particle mixture is from 100 to 250 \( \mu s \) with a step of 50 \( \mu s \); thickness \( H_{ign} \) of the layer in which the combustion wave ignition is initiated - from 10 to 25 \( \mu m \) with a step of 5 \( \mu m \).

Analysis of a large array of simulation results made it possible to determine the characteristics of the SHS process: combustion temperatures, the velocity of the combustion wave front, the quantitative ratio of the synthesized phases for various modes of SHS initiation, etc. Estimates of the characteristics of the SHS process made it possible to determine the ranges of "threshold" values for the parameters of the program model of the procedure for 3D-simulation of SHS macrokinetics (key parameters of the ignition of the SHS reaction):

- the initial temperature \( T_0 \) for preliminary heating of the powder mixture of Ni-Al particles should be at least 600 \( K \), for example, close to a value of about 800 \( K \);
- the temperature \( T_{ign} \) corresponding to the combustion wave ignition in a powder mixture of Ni-Al particles should be in the range of 1300-1500 \( K \);
- the time \( t_{ign} \) corresponding to the time of exposure to the heat pulse until the moment of the combustion wave ignition in the mixture of Ni-Al particles must be at least 0.2 ms (or 200 \( \mu s \));
- the thickness \( H_{ign} \) of the layer in which the combustion wave ignition is initiated during the time \( t_{ign} \) must be at least 20 \( \mu m \), i.e. not less than the thickness of the mesocell shell (thickness of the layer of Al-particles).

Below are graphical illustrations of the simulation results for the values of the four parameters of the program model, taken from the found ranges of their "threshold" values.

**Note 1:** in the legends to figures 3, 5 and 7, a series of values for the number of iterations \( N = (0; 5000; 10000; 15000; 20000; 25000; 100000; 200000; 300000; 400000) \), multiplying by the time step \( \tau = 10^{-8} \text{ s} \), determines a number of values of time moments \( t = (0; 0.05; 0.1; 0.15; 0.2; 0.25; 1; 2; 3; 4) \), expressed in ms.

**Note 2:** along the X-axis in each of figures 4, 6, 8, the number of iterations \( N \) is reduced 1000 times. Therefore, the values of the time counts corresponding to the values of the number of iterations \( N \) on this X-axis are obtained by multiplying by 1000\( t \), where \( \tau = 10^{-8} \text{ s} \). For example, on the X-axis, count 25 \( (N = 25000) \), corresponding to the smallest scale division, will correspond to the time \( t = 0.25 \text{ ms} \) (or 250 \( \mu s \)), which is 0.05 ms more than \( t_{ign} \). The maximum count on the X-axis of 500 \( (N = 500000) \) corresponds to the time \( t = 5 \text{ ms} \) (or 5000 \( \mu s \)).

**Note 3:** when the SHS process is simulated, heat transfer to the external environment was not taken into account in the heat conduction equation, therefore, the CBP-structure cluster is a closed thermodynamic system. Due to the closed nature of the system, the thermal energy released due to the SHS reaction in the CBP-structure cluster is accumulated, and therefore, after equalizing the temperature in its volume, approximately starting from the number of iterations \( N = 100000 \) (time \( t = 1 \text{ ms} \)), the temperature in this volume continues to increase with time. The fact of a further rise in temperature after 1 \( ms \) is confirmed by all three figures (figures 3, 5 and 7).

In figures 3, 5 and 7, the directions “50x50”-direction and “21x21”-direction mean two directions parallel to the Z-axis and outgoing from two points on the XY plane with coordinates, respectively: a)
(X, Y) = (50, 50); b) (X, Y) = (21, 21). The “50x50”-direction passes through the central mesocell, and the “21x21”-direction passes through 1/8 of the lower cornered mesocell, through the edge of the central mesocell, and through 1/5 of the upper cornered mesocell. The central mesocell along the Z-axis occupies the Z-coordinate range from 21 to 121 μm (its center is at a height of 71 μm), and the “core-shell” interface is located at a height of 41 μm. Analyzing figures 3, 4, 5, and 6 for the central mesocell, we can say the following.

For the case \( T_{\text{ign}} = 1300 \) K, according to figure 3, by the time 0.05 ms \((N = 5000)\) at the “core-shell” interface of the central mesocell (in the vicinity of the 41 μm coordinate) the temperature rises to 1127 K, i.e. reaches the melting temperature of the \( \beta \)-phase (NiAl). Therefore, according to figure 4, the thickness of the \( \beta \)-phase initially increased to a greater extent and, to a lesser extent, the thickness of the \( \gamma \)-phase (NiAl), for which the melting temperature is \( T = 1405 \) K. At such temperatures of the SHS process (at \( T < 1127 \) K), the formation of the \( \beta \)-phase and the \( \gamma \)-phase at the interface between “liquid Al - solid Ni” is most natural [5]. After 0.05 ms \((N = 5000)\), the temperature rises above 1127 K and the \( \beta \)-phase rapidly decomposes, and the thickness of the \( \gamma \)-phase interlayer continues to grow rapidly, since the temperature in the SHS combustion wave is still far from its melting temperature 1405 K (see figure 3). In the time range from 3 to 5 ms (from 300000 to 500000 iterations), when the temperature exceeds 1250 K, the higher-temperature \( \delta \)-phase (NiAl) begins to increase slightly (its melting temperature is equal to 1911 K).

For the case of \( T_{\text{ign}} = 1500 \) K, according to figure 5, the temperature in the combustion wave grows faster than in the case of \( T_{\text{ign}} = 1300 \) K, and it reaches the value of 1127 K a little earlier (approximately by the time 0.03 ms). In the initial time interval, at the “core-shell” interface of the central mesocell, similarly to the previous case, the thickness of the \( \beta \)-phase increased to a greater extent, but then it passed into the decay stage. The thickness of the \( \gamma \)-phase (NiAl) continued to grow rapidly, which is confirmed by figure 6. However, after a time instant of the order of 1 ms \((N = 100000)\) iterations, the temperature in the volume of the CBP-structure cluster has already equalized (about 1370 K, figure 5) and continues to grow with time, not yet reaching the melting temperature of the \( \gamma \)-phase (NiAl), equal to 1405 K. This temperature range stimulates the growth of the \( \delta \)-phase (NiAl), which is confirmed by figure 6. By the time instant 2 ms \((N = 200000)\) iterations, the combustion temperature reaches the melting temperature of the \( \gamma \)-phase (1405 K, figure 5), and by the time instant 2.3 ms \((N = 230000)\) iterations, the decay of the \( \gamma \)-phase begins (figure 6) with a more intense increase in the thickness of the \( \delta \)-phase (NiAl).

For four lobes (1/8 each) of the lower cornered mesocells (figure 2(a)), which are partially located from the very beginning in the SHS initiation layer, the diffusion kinetics (figure 8) differs markedly from the diffusion kinetics (figures 4 and 6), occurring in the central mesocell. Namely, the SHS ignition layer transverse to the Z-direction (its thickness is \( H_{\text{ign}} = 20 \) μm) captures most of the volumes of the four lower cornered lobes of mesocells, incl. more than 2/3 of the volumes of the Ni-cores located in the centers of the four lower cornered lobes of the mesocells. Therefore, the initially high temperature (in the range from 1250 to 1300 K, figure 7) in these cornered lobes of the mesocells provides Ni-atoms with a higher diffusion mobility as compared to Ni-atoms in the central mesocell, where the temperature during the time \( t_{\text{ign}} \) is approximately 200 K lower. This SHS mode for cornered mesocells is close to the “thermal explosion” mode upon initiation of SHS and, as is known [8], taking into account the mass content of particles (68.5wt.%Ni, 31.5wt.%Al), the formation of the \( \varepsilon \)-phase (NiAl) is preferable, which is confirmed by figure 8. That is, within the time interval up to \( t_{\text{ign}} = 0.2 \) ms, the thickness of only one \( \varepsilon \)-phase (NiAl) grows at a high rate. Then, at \( t > t_{\text{ign}} \), “free boundary conditions” begin to act, and the temperature in the cornered mesocells decreases slightly. This leads to a decrease in the diffusion mobility of Ni-atoms and, taking into account the above mass contents of Ni and Al particles, the thickness of the \( \delta \)-phase (NiAl) begins to grow, and the thickness of the \( \varepsilon \)-phase (NiAl) decreases. With an increase in the thickness of the \( \delta \)-phase (as a diffusion layer) the mobilities of Ni and Al atoms become equal; therefore, later than the moment of time \( t = 3 \) ms, the growth of the \( \delta \)-phase (NiAl) continues and the \( \varepsilon \)-phase (NiAl) decomposes almost to the end.
Figure 3. A set of temperature profiles for “50x50”-direction in the CBP-structure cluster: $T_0 = 800$ K, $T_{ign} = 1300$ K, $t_{ign} = 0.2$ ms ($N = 20000$), $H_{ign} = 20$ μm.

Figure 4. A set of time dependences of normalized radii for intermetallic phase interlayers in the central mesocell of the CBP-structure cluster: $T_0 = 800$ K, $T_{ign} = 1300$ K, $t_{ign} = 0.2$ ms, $H_{ign} = 20$ μm.
Figure 5. A set of temperature profiles for “50x50” direction in the CBP-structure cluster: \( T_0 = 800 \text{ K}, \ T_{ign} = 1500 \text{ K}, \ t_{ign} = 0.2 \text{ ms} \ (N=20000), \ H_{ign} = 20 \mu \text{m}. \)

Figure 6. A set of time dependences of normalized radii for intermetallic phase interlayers in the central mesocell of the CBP-structure cluster: \( T_0 = 800 \text{ K}, \ T_{ign} = 1500 \text{ K}, \ t_{ign} = 0.2 \text{ ms}, \ H_{ign} = 20 \mu \text{m}. \)
Figure 7. A set of temperature profiles for “21x21”-direction in the CBP-structure cluster: $T_0 = 800$ K, $T_{ign} = 1300$ K, $t_{ign} = 0.2$ ms ($N = 20000$), $H_{ign} = 20\text{ }\mu$m.

Figure 8. A set of time dependences of normalized radii for intermetallic interlayers in the lower cornered mesocells of the CBP-structure cluster: $T_0 = 800$ K, $T_{ign} = 1300$ K, $t_{ign} = 0.2$ ms, $H_{ign} = 20\text{ }\mu$m.
4. Conclusions
Summarizing the above, we present the following main results of the work:

1. the testing of the created software package for 3D-simulation of SHS macrokinetics in a heterogeneous powder system was continued. At the stage of testing the software package, the CBP-structure cluster (the model cluster of a “closest ball 3D-packing of mesocells”) was used to study the processes of SHS temperature macrokinetics and diffusion kinetics in mesocells;

2. the parameters of the program model of the procedure for 3D-simulation of SHS macrokinetics (key parameters of the SHS reaction ignition) were determined:
   - the initial temperature $T_0$ for preliminary heating of the powder mixture of Ni-Al particles should be at least 600 K, for example, close to a value of about 800 K;
   - the temperature $T_{ign}$ corresponding to the combustion wave ignition in a powder mixture of Ni-Al particles should be in the range of 1300-1500 K;
   - the time $t_{ign}$ corresponding to the time of exposure to the heat pulse until the moment of the combustion wave ignition in the mixture of Ni-Al particles must be at least 0.2 ms (or 200 μs);
   - the thickness $H_{ign}$ of the layer in which the combustion wave ignition is initiated during the time $t_{ign}$ must be at least 20 μm, i.e. not less than the thickness of the mesocell shell (thickness of the layer of Al-particles).

3. the results of computational experiments have shown that the diffusion kinetics is interrelated with the temperature kinetics and is nonuniform in mesocells with different locations within the CBP-structure cluster. Inhomogeneity of diffusion kinetics leads to inhomogeneity of the formation of intermetallic phases in various mesocells of the CBP-structure cluster.

References
[1] Jordan V, Loktionov A 2011 Proc. of Conf. “Modeling of nonequilibrium systems” (Krasnoyarsk: “IPK SFU” Publisher) pp 98-104
[2] Jordan V, Belov T 2012 Proc. of Conf. “Information Technology and Mathematical Modeling” vol 1 (Kemerovo: “Praktika” Publisher) pp 45-50
[3] Jordan V I, Shmakov I A and Grigorevskaya A A 2021 Journal of Physics: Conference Series 1745 012062. doi:10.1088/1742-6596/1745/1/012062
[4] Jordan V I 2011 Izvestiya of the Altai State University. Physics series 69(1/2) 154-158
[5] Kovalev O, Belyaev V 2013 Combustion, Explosion, and Shock Waves 49(5) 64-76
[6] Jordan V I, Shmakov I A and Kurgumbaev M E 2015 Proc. of Conf. “Mathematics and its applications: fundamental problems of science and technology” (Barnaul: “AltGU” Publisher) pp 264-272
[7] Panchenko Ju A and Jordan V I 2018 High-Performance Computing Systems and Technologies 2(2) 54-62
[8] Lapshin O V, Ovcharenko V E and Boyangin E N 2002 Combustion and explosion physics 38(4) 59-64