3D computer-aided simulation of SHS macrokinetics in the Ni-Al porous medium with the closest packing of “mesocells”

V I Jordan, I A Shmakov, A A Grigoryevskaya

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

Abstract. The paper discusses the methodological features of the procedure for simulation the SHS process in the "etalon" model structure of the closest packing of the so-called mesocells in the form of balls of the same radius. In the center of the mesocell there is a spherical Ni particle (radius \(R_{Ni} = 30 \mu m\)), around which aluminum particles of radius \(R_{Al} = 10 \mu m\) are contained in a spherical interlayer with a thickness of 20 \(\mu m\). The etalon structure is formed by a program that takes into account the distribution of mesocells in the structure of the closest packing (alternating flat layers with square symmetry). The software has implemented the procedure for preparing the “calculation area” in the form of a three-dimensional grid of nodal points (3D Cartesian calculation grid with the same step \(h = 1 \mu m\) along the \(x, y, z\) coordinates), for which a 3D data structure Points\([i][j][k]\) with several record fields was created. The record fields of the structure Points\([i][j][k]\) are the following: \(T\) - temperature, \(\eta\) - depth of chemical conversion, type - type of material and etc. A technique for numerical solution of the heat conduction equation using an implicit scheme of bicyclic splitting based on the symmetric Krank-Nicholson scheme is implemented. Together with the bicyclic splitting scheme, a procedure is implemented for numerically solving the diffusion kinetics equation in mesocells. For computational speedup, the parallelization schemes of cycles are used, which determine the main time costs for performing “runs (sweep)” in the computing schemes. As a result of 3D simulation of SHS macrokinetics, sets of temperature profiles and time-varying relative radii (external boundaries) of intermetallic phase layers in mesocells are given.

1. Introduction
Self-propagating high temperature synthesis (SHS) is an effective method for producing modern functional materials with desired properties. In the SHS process, under the influence of a heat pulse in a mixture of finely dispersed powders, an intense exothermic combustion reaction occurs in a small layer and the combustion wave propagates along the entire sample by heat transfer from layer to layer. The properties of SHS products largely depend on the initial structure of the packing of particles of the reacting mixture and other reaction parameters. The powder mixture is practically a porous spatially inhomogeneous medium with a specific structure of the packing of reagent particles. Using the previously developed program [1, 2], it is possible to generate various particle packing structures from various materials (for example, Ni, Al particles, etc.) with different sizes and coordinates of filling the volume of the powder mixture (with given statistical distributions).
Analyzing computational experiments on the generation of packing structures using this program, it was found that the average porosity of such structures (with spherical particles) practically turns out to be at least 40% (porosity from 40 to 70%). To a greater extent, such values of the porosity of the packing structure correspond to the so-called "piled up density" of the mixture of particles. A lower level of porosity (30% or less) is achieved by "prepressing" the mixture. Therefore, as a "test" denser structure of the particle packing, it was decided to implement a "test" dense packing structure with a high “symmetry” of particle arrangement and a relative filling density of the SHS sample volume of 70% (porosity about 30%). Such a dense packing structure was used to test the developed software package for the study of macrokinetics of SH-synthesis.

The aim of this work is to develop the algorithmic foundations and a software package for mathematical simulation and study of the macrokinetics of SH-synthesis of intermetallic compounds in binary systems such as Ni-Al and Ti-Al (taking into account discrete-continuous representations of the structure of the initial mixture and the structure of formation intermetallic phases in a reacting medium). To test the software package, computational experiments were performed.

2. Methodological and algorithmic principles of 3D simulation of the SHS macrokinetics in a medium with the closest packing of “mesocells”

The system of equations of the SHS process consists of the heat conduction equation (1) with the function of exothermic heat release (2) and the kinetics equation (3) with the kinetic function of homogeneous kinetics (4) for single-phase regions (Ni3Al, NiAl, etc.).

\[
\frac{\partial T}{\partial t} = \text{div} (\alpha \cdot \text{grad}(T)) + f(T, \eta), \tag{1}
\]

\[
f(T, \eta) = \left(\frac{Q}{C_{\text{spec}}}\right) \cdot k(T) \cdot \varphi(\eta) + \beta \cdot (T - T_0), \tag{2}
\]

\[
\frac{\partial \eta}{\partial t} = k(T) \cdot \varphi(\eta) = G(T, \eta), \tag{3}
\]

\[
\varphi(\eta) = (1 - \eta)^n, \tag{4}
\]

where \(T = T(x, y, z, t)\) is the temperature at the current calculated spatial point of the mixture at time \(t\); \(\alpha=\lambda/(C_{\text{spec}} \cdot \rho)=\alpha(x, y, z, T)\) and \(\lambda=\lambda(x, y, z, T)\) - respectively, thermal diffusivity and thermal conductivity of the mixture component; \(T_0\) is the temperature of the environment; \(T_{\text{ign}}\) is the ignition temperature (self-ignition) of the SHS sample; \(C_{\text{spec}}=c(x, y, z, T)\) and \(\rho=\rho(x, y, z, T)\) - respectively, specific heat and density in the vicinity of the calculated point; \(Q = \dot{Q}(x, y, z, T)\) is the thermal effect of the reaction per unit mass of the product, taking into account stoichiometry of the composition of the components in the vicinity of the calculated point; \(\eta=\eta(x, y, z, t)\) is the depth of the chemical conversion (mass fraction of the product relative to the mass of the reaction mixture and the product); \(\beta\) - coefficient taking into account heat loss to the environment.

It should be noted that often “in the first approximation” the temperature dependence of the parameters \(\alpha, \lambda, c \) and \(\rho\) is neglected. However, for a wide range of temperature changes \(T(x, y, z, t)\), such neglect is not justified and the approach proposed by the authors takes into account the inhomogeneity of thermophysical parameters and the discreteness of the porous medium.

Initial conditions (except for the boundary \(z = 0\)): \(T(x, y, z, 0) = T_0\), at the boundary \(z = 0\) at first \(T(x, y, 0, 0) = T_{\text{ign}}\), and after a while - “free” boundary conditions of the first kind. The Arrhenius temperature-activation function has the form: \(k(T) = k_0 \cdot \exp (-E/(R \cdot T))\), where \(k_0\) is the pre-exponent and \(E = E(x, y, z, T(x, y, z, t))\) is the reaction activation energy corresponding to the phase of the product.

The authors developed and programatically implemented the procedure for creating a “etalon” model structure of the closest packing (alternating flat layers with square symmetry, figure 1) of the so-called mesocells in the form of balls of the same radius \((R = 50 \mu m)\) forming a regular structure in the form of a parallelepiped with certain symmetry properties of the arrangement of particles. To describe the structure of the closest packing of mesocells (space filling factor \(\approx 70%\)) in figure 1, the
following parameters are used: M — number of flat layers; N is the number of mesocells located along each of the two directions X and Y in a layer with square symmetry (for odd layers, the value of N is 1 greater than for even ones).

**Figure 1.** 3D closest cubic packings (CCP): 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) the simplest cluster of CPP packing for 3D computing simulation of SHS macrokinetics.

In odd layers, the X- and Y-coordinates of the ball centers corresponding to each other coincide, and in the even layers, the X- and Y-coordinates of the ball centers are displaced in both coordinates relative to the balls of the odd layers by the radius of the ball $R_i$.

When testing the SHS simulation software package developed by the authors in the "etalon" model structure of the closest packing, the odd layers contain 36 balls (6x6), and the even layers contain 25 balls (5x5). Along the Z-coordinate, this structure contains 18 pairs of layers (18 alternating layers with odd and even numbers, respectively). As a result, the etalon model structure (in the form of a parallelepiped) contains 1098 mesocells. In all layers in the central voids of each square of 4 balls, cubic structures of 8 aluminum balls of smaller radius $R_{Al} = 10 \mu m$ are placed (two layers in the form of squares of 4 balls on top of each other). In addition, the structure of 1098 mesocells is additionally "truncated" by the lower horizontal and 4 lateral faces-planes passing through the centers of the lower 4 corner mesocell spheres and by the upper horizontal plane touching the mesocell spheres of the last 18th even layer. That is, the corner balls-mesocells after truncation look like the corner balls shown in figure 1(d). Thus, the dimensions of the etalon structure along the X and Y axes are equal to 500 μm (from the center of the 1st to the center of the 6th ball), and about 2500 μm along the Z axis.

The procedure for preparing the "computational domain" in the form of a three-dimensional grid of nodal points was programmed with the aim to solve equations (1)-(4) using "grid" computational schemes (in this paper, based on Crank-Nicholson schemes). 3D Cartesian calculation grid have the same step $h = 1 \mu m$ along the x, y, z coordinates (the number of points is 62500000 = 500x500x2500). The software package is implemented in C ++ using the GCC-8 compiler, as well as using the OpenMP and MPICH 3.1.3 parallel programming systems running GNU/Linux. The data structure Points[i][k][l] corresponds to the 3D computational grid. The data structure Points[i][k][l] have three fields: Points[i][k][l].type; Points[i][k][l].t; Points[i][k][l].eta, where type is the type of material, t is the temperature, eta is the conversion depth. For each point these fields of the Points[i][k][l] structure are used in current calculations and in each subsequent time layer (at each $(j+1)$th iteration), at least the temperature and conversion depth fields change in the result of the recount (the type of material at some iterations may also vary).

Prior to the start of the SHS reaction, a spherical nickel particle Ni of radius $R_{Ni} = 30 \mu m$ is located in the center of each mesocell of radius $R_s = 50 \mu m$, around which aluminum particles of radius $R_{Al} = 10 \mu m$ are contained in the spherical interlayer (figure 2(a)). During the SHS reaction, with increasing temperature in the mesocells, diffusion layers of intermetallic compounds are formed on the surfaces of central Ni particles (figure 2(b)), separating the Ni particle and the Al particle layer. Al particles at a temperature above the melting point of 933 K form a monolithic melt layer, as shown in figure 2(b).
Therefore, the radius \( r_i(T) \) of the phase interlayers is determined by the kinetic function (4) of homogeneous kinetics. Then, in the temperature-activation function of Arrhenius \( k(T) = k_0 \exp (-E/(R \cdot T)) \) in each phase layer (with known restrictions on the radii \( r_{i-1} \) and \( r_i \)), we can take

\[
\begin{align*}
C_i = A_i/r + B_i,
\end{align*}
\]

The radii of the phase layers are fixed, therefore, the index \( i \) in the equations can take the values \( i = 2, 3, 4, 5 \), which corresponds to the phases: 1 - Ni, 2 - \( \varepsilon \) (Ni3Al), 3 - \( \delta \) (NiAl), 4 - \( \gamma \) (Ni3Al3), 5 - \( \beta \) (NiAl3), 6 - Al. The radii of the phase layers are indicated as \( r_i(t) \). Therefore, the radius \( r_6 = R_9 \).

Substituting in (6) the stationary solutions of equation (5): \( C = A/r + B \), we obtain a system of ordinary differential equations (4):

\[
\begin{align*}
d_i \frac{d r_i}{d t} = -\theta_{i+1} \frac{r_{i+1}}{r_i \cdot (r_i - r_{i+1})} + \theta_i \frac{r_{i+1}}{r_i \cdot (r_i - r_{i-1})},
\end{align*}
\]

where \( d_i = C_{i+1}^+ - C_i^+ \), \( \theta_i = D_i(T) \cdot (C_{i+1}^+ - C_i^+) \), \( i = 1, 2, 3, 4 \).

The radii of homogeneous phase interlayers (figure 2(b)), which vary in time, are determined by the Runge-Kutta method from equation (7). When solving the heat conduction equation in phase interlayers, the kinetic function (4) of homogeneous kinetics is used. Then, in the temperature-activation function of Arrhenius \( k(T) = k_0 \exp (-E/(R \cdot T)) \) in each phase layer (with known restrictions on the radii \( r_{i-1} \) and \( r_i \)), we can take into account the diffusion problem in the mesocell being solved, as a result of which the changed radii of intermetallic layers (Ni3Al, NiAl, etc.) are fixed, determine the reaction volumes of heat emission and which are used in the numerical solution of the heat conduction equation using the implicit bicyclic splitting scheme based on the symmetric Crank-Nicholson scheme (see below). In each mesocell, the numerical solution of the problems of reaction diffusion is carried out independently of each other and is therefore easily parallelized by independent computational processes (parallelism of tasks). A brief summary of the methodology for solving the diffusion problem in the mesocell is given below.

The problem of diffusion kinetics based on the numerical solution of the diffusion equations and balance relations at moving interphase boundaries [4, 5] is solved in each mesocell:

\[
\begin{align*}
\frac{1}{D_i} \frac{\partial C_i}{\partial t} = \frac{\partial^2 C_i}{\partial r^2} + \frac{2}{r} \frac{\partial C_i}{\partial r},
\end{align*}
\]

where \( C_i \) is the mass concentration of nickel in the \( i \)-th phase, \( D_i(T) = k_i \exp (-E/(R \cdot T)) \) is the mutual diffusion coefficient in the \( i \)-th layer, \( C_{i-1}^+(T), C_i^-(T) \) are the dependences of the equilibrium concentrations on temperature, given from state diagrams (boundaries of phase concentration regions). The number of layers (intermediate phases) depends on the type of system under consideration, therefore, the index \( i \) in the equations can take the values \( i = 2, 3, 4, 5 \), which corresponds to the phases: 1 - Ni, 2 - \( \varepsilon \) (Ni3Al), 3 - \( \delta \) (NiAl), 4 - \( \gamma \) (Ni3Al3), 5 - \( \beta \) (NiAl3), 6 - Al. The radii of the phase layers are indicated as \( r_i(t) \). Therefore, the radius \( r_6 = R_9 \).

At each \((j+1)\)-th time iteration within each spherical mesocell, the diffusion kinetics task [2] is solved, as a result of which the changed radii of intermetallic layers (Ni3Al, NiAl, etc.) are fixed, determine the reaction volumes of heat emission and which are used in the numerical solution of the heat conduction equation using the implicit bicyclic splitting scheme based on the symmetric Crank-Nicholson scheme (see below). In each mesocell, the numerical solution of the problems of reaction diffusion is carried out independently of each other and is therefore easily parallelized by independent computational processes (parallelism of tasks). A brief summary of the methodology for solving the diffusion problem in the mesocell is given below.

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account the corresponding constant $k_0$, activation energy $E_a$, etc. In addition, in each phase layer, the corresponding temperature value, calculated when solving the heat equation, is taken into account. In the entire volume of the SHS sample, the temperature profile $T(x, y, z, t_{j+1})$ is calculated for each $(j+1)$-th moment of time $t_{j+1}$ (for each $(j+1)$-th time layer) after calculation values of the radii $r_i(t_{j+1})$ in steps of time $\tau = 10^{-8}$ c. The following is a procedure for solving the grid equations of heat conduction (1) and kinetics (3) in which grid schemes are obtained that correctly use the discontinuity property of the first kind of thermophysical and other parameters at the interfaces of different media (various particles).

In [6], an implicit bicyclic splitting scheme was derived based on the symmetric Crank–Nicholson scheme, which uses the separation (“splitting”) of the time layer into 7 intermediate time layers and on the basis of which 8 equations are derived below. The first three equations (8)-(10), corresponding to the $x, y, z$-directions and simultaneously the $i, j, k$-indices, as well as the last three equations (14)-(16), corresponding in the opposite order to the $z, y, x$-directions and simultaneously the $l, k, i$-indices, are solved sequentially each time according to one of the three indicated indices by a one-dimensional “sweep” method nested in 2-dimensional cycles according to the remaining indices. These 2-dimensional nested loops are fairly easy to parallelize.

\[
A^{j+1/2}_{i,k,l} T^{j+1/2}_{i,k,l} - C^{j+1/2}_{i+k,l} T^{j+1/2}_{i+k,l} + B^{j+1/2}_{i+l,k} T^{j+1/2}_{i+l,k} = -F^{j+1/2}_{i+l,k,i},
\]

where \( A^{j+1/2}_{i,k,l} = \frac{\tau}{4h^2} a^{j+1/2}_{i,k,l} \); \( C^{j+1/2}_{i+k,l} = \left[ 1 + \left( \alpha^{j+1/2}_{i+k,l} + \alpha^{j+1/2}_{i+l,l} \right) \frac{\tau}{4h^2} \right] \); \( B^{j+1/2}_{i+l,k} = \frac{\tau}{4h^2} a^{j+1/2}_{i+l,k,l} \);

\[
F^{j+1/2}_{i+l,k,i} = A^{j+1/2}_{i+k,l} T^{j+1/2}_{i+k,l} + D^{j+1/2}_{i+l,k} T^{j+1/2}_{i+l,k} + B^{j+1/2}_{i+l,k} T^{j+1/2}_{i+l,k};
\]

\[
D^{j+1/2}_{i+l,k} = \left[ 1 - \left( \alpha^{j+1/2}_{i+k,l} + \alpha^{j+1/2}_{i+l,k} \right) \frac{\tau}{4h^2} \right];
\]

\[
A^{j+2/2}_{i,k,l} T^{j+2/2}_{i,k,l} - C^{j+2/2}_{i+k,l} T^{j+2/2}_{i+k,l} + B^{j+2/2}_{i+l,k} T^{j+2/2}_{i+l,k} = -F^{j+2/2}_{i+l,k,i},
\]

where \( A^{j+2/2}_{i,k,l} = \frac{\tau}{4h^2} a^{j+2/2}_{i,k,l} \); \( C^{j+2/2}_{i+k,l} = \left[ 1 + \left( \alpha^{j+2/2}_{i+k,l} + \alpha^{j+2/2}_{i+l,k} \right) \frac{\tau}{4h^2} \right] \); \( B^{j+2/2}_{i+l,k} = \frac{\tau}{4h^2} a^{j+2/2}_{i+l,k,l} \);

\[
F^{j+2/2}_{i+l,k,i} = A^{j+2/2}_{i+k,l} T^{j+2/2}_{i+k,l} + D^{j+2/2}_{i+l,k} T^{j+2/2}_{i+l,k} + B^{j+2/2}_{i+l,k} T^{j+2/2}_{i+l,k};
\]

\[
D^{j+2/2}_{i+l,k} = \left[ 1 - \left( \alpha^{j+2/2}_{i+k,l} + \alpha^{j+2/2}_{i+l,k} \right) \frac{\tau}{4h^2} \right];
\]

\[
A^{j+1/2}_{i,k,l} T^{j+1/2}_{i,k,l} - C^{j+1/2}_{i+k,l} T^{j+1/2}_{i+k,l} + B^{j+1/2}_{i+l,k} T^{j+1/2}_{i+l,k} = -F^{j+1/2}_{i,k,l,i},
\]

where \( A^{j+1/2}_{i,k,l} = \frac{\tau}{4h^2} a^{j+1/2}_{i,k,l} \); \( C^{j+1/2}_{i+k,l} = \left[ 1 + \left( \alpha^{j+1/2}_{i+k,l} + \alpha^{j+1/2}_{i+k,l} \right) \frac{\tau}{4h^2} \right] \); \( B^{j+1/2}_{i+l,k} = \frac{\tau}{4h^2} a^{j+1/2}_{i+l,k,l} \);

\[
F^{j+1/2}_{i,k,l,i} = A^{j+1/2}_{i+k,l} T^{j+1/2}_{i+k,l} + D^{j+1/2}_{i+k,l} T^{j+1/2}_{i+k,l} + B^{j+1/2}_{i+l,k} T^{j+1/2}_{i+l,k};
\]

\[
D^{j+1/2}_{i+k,l} = \left[ 1 - \left( \alpha^{j+1/2}_{i+k,l} + \alpha^{j+1/2}_{i+k,l} \right) \frac{\tau}{4h^2} \right].
\]

The equation of the fourth intermediate time layer of the circuit requires estimates $\dot{\eta}^{j+1/2}_{i,k,l}$ and $\dot{\tilde{T}}^{j+1/2}_{i,k,l}$, which can be obtained by a self-consistent cyclic process as follows.

We initialize $\dot{\tilde{T}}^{j+1/2}_{i,k,l} = T^{j+1/2}_{i,k,l}$. Then a self-consistency cycle is performed with a certain "threshold" for the accuracy of convergence of the estimates of the quantities $\dot{\eta}^{j+1/2}_{i,k,l}$ and $\dot{T}^{j+1/2}_{i,k,l}$ to their limiting values:
\begin{equation}
\left\{ \begin{array}{c}
\dot{\eta}_{i,k,l}^{j+1/2} = \eta_{i,k,l}^{j} + \frac{\tau}{2} G \left( \hat{T}_{i,k,l}^{j+1/2}, \eta_{i,k,l}^{j} \right), \\
\dot{\hat{T}}_{i,k,l}^{j+1/2} = T_{i,k,l}^{j} + \frac{\tau}{2} f \left( \hat{T}_{i,k,l}^{j+1/2}, \eta_{i,k,l}^{j+1/2} \right)
\end{array} \right. ,
\end{equation}

As a result of a certain number of iterations, estimates of $\eta_{i,k,l}^{j+1/2}$ and $\hat{T}_{i,k,l}^{j+1/2}$ will be achieved with the necessary accuracy.

The equation of the fifth intermediate time layer of the circuit has the form:
\begin{equation}
T_{i,k,l}^{j+5/8} = T_{i,k,l}^{j+3/8} + \tau f \left( T_{i,k,l}^{j+1/2}, \eta_{i,k,l}^{j+1/2} \right)
\end{equation}

The computational scheme for calculating the "conversion depth" has the form:
\begin{equation}
\eta_{i,k,l}^{j+1} = \eta_{i,k,l}^{j} + \tau G \left( \hat{T}_{i,k,l}^{j+1/2}, \eta_{i,k,l}^{j+1/2} \right)
\end{equation}

Below are the schemes for the 6-th, 7-th intermediate layers in time and for the “final” (j+1)-th time layer.
\begin{equation}
A_{i,k,l}^{j+1/2} = \frac{\tau}{4h^2} a_{i,k,l}^{j+1/2}; \quad C_{i,k,l+1}^{j+1/2} = \left[ 1 + \left( a_{i,k,l}^{j+1/2} + a_{i,k+1,l}^{j+1/2} \right) \frac{\tau}{4h^2} \right] ; \quad B_{i,k,l+1}^{j+1/2} = \frac{\tau}{4h^2} a_{i,k+1,l}^{j+1/2}; \\
F_{i,k,l+1}^{j+5/8} = A_{i,k,l}^{j+1/2} T_{i,k-l,l}^{j+5/8} + D_{i,k,l+1}^{j+1/2} T_{i,k+l+l}^{j+5/8} + B_{i,k+1,l}^{j+1/2} T_{i,k+l-l}^{j+5/8}; \quad D_{i,k,l+1}^{j+1/2} = \left[ 1 - \left( a_{i,k,l}^{j+1/2} + a_{i,k+1,l}^{j+1/2} \right) \frac{\tau}{4h^2} \right]
\end{equation}

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F_{i,k+l+1}^{j+5/8} = A_{i,k,l}^{j+1/2} T_{i,k-l,l}^{j+5/8} + D_{i,k+1,l}^{j+1/2} T_{i,k+l-l}^{j+5/8} + B_{i,k+1,l}^{j+1/2} T_{i,k+l-l}^{j+5/8}; \quad D_{i,k+l+1}^{j+1/2} = \left[ 1 - \left( a_{i,k,l}^{j+1/2} + a_{i,k+1,l}^{j+1/2} \right) \frac{\tau}{4h^2} \right]
\end{equation}

3. Testing the software package and the results of computational experiments
The methodological and algorithmic principles of 3D modeling of the SHS macrokinetics in an environment with the closest packing of “mesocells” are implemented in the form of a software package. When testing the software package based on computational experiments, the stability conditions of computational grid schemes were determined and test calculations were performed for the “etalon” model structure of the closest packing (figure 1(d) - the simplest cluster of CPP packing for 3D computing simulation of SHS macrokinetics). Figure 3 shows the sets of temperature profiles.
along two directions parallel to the Z-axis. In the first, the X- and Y-coordinates of all direction points are equal to each other and equal to 21 μm, in the second, the X- and Y-coordinates of all direction points are equal to each other and equal 50 μm.

**Figure 3.** A set of temperature profiles (temperature distributions along the two directions of the SHS-sample: (21, 21, Z) and (50, 50, Z)) at different time points: the initial temperature of the entire SHS sample is 600 K; the ignition temperature for SHS-sample is 1200 K.

The first direction passes through two corner mesocells, which correspond to 1/8 of a fraction of the whole mesocell (figure 1(d) – the simplest cluster of CPP packing).

The second direction passes through the central full mesocell. Until the SHS ignition, the entire sample was heated to a temperature of 600 K, and the ignition temperature for a flat boundary (z = 0) was set to 1200 K. It should be noted that the heat release function (2) in equation (1) is enabled (active) only at the 3D Cartesian calculation grid points located in the phase layers \( i = 2, 3, 4, 5 \) (2 - \( \varepsilon \) (Ni3Al), 3 - \( \delta \) (NiAl), 4 - \( \gamma \) (Ni2Al3), 5 - \( \beta \) (NiAl3)). At the grid points located in the layers Ni (\( i = 1 \)) and Al (\( i = 6 \)), the heat release function (2) is disabled (inactive, equal to zero). In other words, in the “pure” layers of Ni and Al, there is no exothermic heat release reaction.

As can be seen from figure 3, approximately by the end of the first millisecond of the SHS process, the combustion wave passed the length of the design cluster of 170 μm with the velocity of the combustion front approximately equal to 0.17 m/s (or 17 cm/s). In the book [7] for similar values of the particle mass contents (68.5wt.%Ni, 31.5wt.%Al) experimental values of the combustion velocity are given in the range from 0.12 to 0.2 m/s, covering the simulation result. Along its entire length, a “temperature plateau” is established (figure 3), the value of which is slightly higher than the ignition temperature of 1200 K. At the end of the first direction (21, 21, Z), the temperature reaches 1206.54 K, and at the end of the second direction (50, 50, Z), it reaches 1206.34 K. A slight difference in temperature values can be explained by the difference in thermophysical properties at different points of the inhomogeneous medium. An increase in the combustion temperature (up to approximately 1500-1600 K) can be achieved by increasing the ignition temperature above 1200 K (in our case, it is 1200 K) and by increasing the pre-exponent \( k_0 \) in the Arrhenius function \( k(T) \). The pre-exponent \( k_0 \) in computational experiments was 10^7.
The results of simulation the process of diffusion kinetics in various mesocells can be analyzed in figures 4 and 5.

Figure 4. Kinetics of changes in the relative radii (external boundaries) of the intermetallic phase interlayers (Ni, ε, δ, γ, β) in the mesocell located in the lower corner of the cluster (1/8 of the total volume of mesocell, figure 1(d)).

Figure 4 shows the time dependences of the relative radii of the intermetallic interlayers (outer boundaries of the interlayers) in the lower corner mesocell (figure 1 (d): 1/8 of the total volume of the mesocell) in contact with the ignition plane of the SHS cluster (z=0). Figure 5 shows similar dependences for the central full mesocell, which is separated from the ignition plane (z=0) at a certain height. The relative radii of the intermetallic interlayers (i=1, 2, 3, 4, 5) were obtained by normalizing the absolute radii to the mesocell radius $R_s$.

The thicknesses of the intermetallic phases (interlayers) formed during the SH-synthesis are determined by the difference in the radii of the neighboring phases. As can be seen from figures 4 and 5, during the first millisecond, the thickness of the β-phase (NiAl$_3$) increases to a greater extent and, to a lesser extent, the thickness of the γ-phase (Ni$_2$Al$_3$). The thickness of each from the remaining phases increases still to a lesser extent. At the same time, in the process of SHS in the mesocells the temperature rises. After the combustion temperature of the β-phase melting point ($T$=1127 K) is reached, the boundary between the Al layer and the β-phase ceases to be mobile (the radius of the β-phase remains unchanged afterwards), and in the β-phase layer begins hers decomposition. At the same time, the thickness of the γ-phase continues to increase and at a certain time, the decomposition of the β-phase is completed (the radius of the γ-phase is compared with the radius of the β-phase and continues to increase). As can be seen from figures 4 and 5, the thickness of the δ-phase (NiAl) continues to grow very slowly. Since the combustion temperature reaches a “plateau” and turns out to be slightly more than 1200 K, which is noticeably less than the melting point of the growing γ-phase ($T$=1405 K), therefore, her boundary remains mobile. At a combustion temperature close to 1200 K, the γ-phase (Ni$_2$Al$_3$) is formed to a large extent and the δ-phase (NiAl) is formed to a small extent.

The dependency graphs in figure 5 are similar to the graphs displayed in figure 4. Since in the central mesocell, which is distant from the ignition plane (z=0), the temperature rise lags behind the temperature rise in the lower corner mesocell in contact with the ignition plane, therefore, the “kinks” in the graphs of figure 5 are shifted to the right relative to similar “kinks” in figure 4.
Figure 5. Kinetics of changes in the relative radii (external boundaries) of the intermetallic phase interlayers (Ni, ε, δ, γ, β) in the mesocell located in the center of the cluster (figure 1(d)).

Figure 6. A set of temperature profiles (temperature distribution along the central direction of the SHS-sample) at different points in time: the initial temperature of the entire SHS sample is 300 K; the ignition temperature of the SHS-sample is 1500 K.

The following is another example of a test calculation of temperature profiles at different points in time (shown in figure 6) for a densely packed mixture of particles (pore size less than 1 μm): the particle size of Ni and Al is the same and equal to 1 μm. A given version of the SHS mixture of particles can be considered practically a model of a “quasi-continuous” medium with a large value of
the “specific” contact surface of particles Ni and Al. SHS initiation (ignition) mode: initial temperature of the entire SHS mixture is 300 K; the ignition temperature of the SHS mixture is 1500 K. In a qualitative sense, the temperature profiles correspond to theoretical concepts, and superadiabatic temperature peaks are observed in the combustion front.

The velocity of the combustion front can be estimated at approximately 11 m/s (almost two orders of magnitude higher than the experimental values). Such an excess of the combustion velocity can be explained by a similar excess of the specific surface of the model “quasi-continuous” medium over the specific surface of the real porous SHS mixture. Simulation of SH-synthesis in nano- and microsized atomic systems Ni-Al with a similar specific contact surface using the LAMMPS package (molecular dynamics method) gives values of combustion velocity [8-11] comparable in order of magnitude with the case considered here (figure 6). A consequence of this is the high combustion temperature in the model “quasi-continuous” medium in the range from 2200 to 2400 K (figure 6). The pre-exponent $k_0$ in computational experiments was equal $2 \times 10^8$. The sufficiently high pre-exponent value $k_0 = 2 \times 10^9$ also affected the high value of the combustion temperature in the range from 2200 to 2400 K (the value of pre-exponent $k_0$ in this case should have had a smaller value).

3. Conclusion
Summarizing the above, we give the following main results of the work:
- is implemented a software package for 3D simulation of SHS macrokinetics in a medium with the closest packing of “mesocells” and studying the process of diffusion kinetics in mesocells;
- stability conditions for computational grid circuits were determined and test calculations were performed for the “etalon” model structure of the closest packing (alternating flat layers with square symmetry, figure 1);
- during further testing, various parameters of the mathematical model of the SHS process will be clarified to ensure agreement between the calculated data and experimental data from various literature sources. For example, for each composition of the components of the SHS mixture (Ni-Al, Ti-Al, etc.), it is necessary to specify (to select) the value of the pre-exponent $k_0$.

Computer simulation of SH-synthesis of intermetallic compounds of Ni-Al system by the software package using parallel computations was carried out on the cluster of workstations (15 PCs) - local area network. Each PC has a 4-core Intel i5-7400 processor, 4 GB RAM.

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