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MODELING OF TEMPERATURE FIELDS OBTAINED BY FORMATION OF COATINGS UNDER NON-STATIONARY TEMPERATURE CONDITIONS

Modeling of temperature fields obtained during the formation of coatings under nonstationary temperature conditions is considered. In this paper, the kinetics of interaction and heat release in a wave is described using the Haikin-Merzhanov model. This is a model of the reaction cell, which is closest in thermokinetic and diffusion processes under non-stationary temperature conditions. Numerical calculations are performed in the following order. First, the kinetic equation by the Runge-Kutta method of the 4th order of accuracy is solved. Then, after the calculated value of $d\eta/dt$ at each point, the initial term F is calculated, which is included in the equation of thermal conductivity and, accordingly, in its divergent form. After that, the numerical solution of the equations of thermal conductivity and diffusion is carried out. The difference equations are nonlinear: the density, heat capacity and thermal conductivity at all points depend on the temperature. Therefore, their linearization is performed: when moving to a new (j + 1) -th time layer, these coefficients at all points are calculated using the temperature values on the j-th layer θ_i^j ; in particular, value $\overline{\lambda}_{i\pm1/2}$. Depending on the type of boundary conditions at ($x_1 = 0$) the first pair of run coefficients is calculated: i. Then the forward run is performed: $P_{1½}$ і $R_{1½}$. Then the forward run is performed: the run coefficients at the points i = 2 ,..., N–1. After that, the formulas determine the temperature values on the new, (j + 1)-th layer over time at the pointi = N (θ_N^{j+1}). After that, the run back is performed: the value of temperature at all points (j + 1) of the th layer is calculated by the expression: θ_{i-1}^{j+1}, i = N–1 ,..., Thus, the developed difference scheme is a scheme of end-to-end calculation.

***Keywords**: non-stationary temperature conditions; boundary conditions; temperature fields; diffusion; protective coatings; nonlinear nonstationary equation.*

Розглянуто моделювання температурних полей отриманих при формуванні покриттів при нестаціонарних температурних умовах. В роботі кінетика взаємодії і тепловиділення в хвилі описується з використанням моделі Хайкіна-Мержанова. Це модель реакційної комірки, яка найбільш близька по термокінетичним та дифузійним процесам при нестаціонарних температурних умовах. Чисельні розрахунки проводяться в наступному порядку. Спочатку вирішується кінетичне рівняння методом Рунге-Кутта 4-го порядку точності. Потім після розрахованого значення $d\eta/dt$ в кожній точці обчислюється початковий член F, який входить до рівняння теплопровідності і, відповідно, в його дивергентну форму. Після цього здійснюється чисельне рішення рівнянь теплопровідності та дифузії. Різницеві рівняння є нелінійними: щільність, теплоємність та коефіцієнт теплопровідності у всіх точках залежать від температури. Тому виконується їх лінеаризація: при переході на новий (j + 1)-й часовий шар ці коефіцієнти у всіх точках розраховуються, використовуючи значення температури на j-му шарі θ_i^j ; зокрема, значення $\overline{\lambda}_{i\pm1/2}$. В залежності від типу граничних умов при $x_1 = 0$ обчислюється перша пара прогоночних коефіцієнтів: $P_{1½}$ і $R_{1½}$. Потім виконується прогін вперед: обчислюються прогоночні коефіцієнти в точках i = 2 ,..., N–1.

Після цього за формулами визначаються значення температури на новому, (j+1)-му шарі за часом в точці i = N (θ_N^{j+1}). Після цього виконується прогін назад: за виразом обчислюються значення температури у всіх точках (j+1)-ого шару: θ_{i-1}^{j+1}, i = N–1 ,..., Таким чином, розроблена різницева схема є схемою наскрізного розрахунку.

***Ключові слова**: нестаціонарні температурні умови; граничні умови; температурні поля; дифузія; захисні покриття; нелінійне нестаціонарне рівняння.*

Problem's Formulation

Analysis of trends in the development of materials in the world, the development of new structural materials with coatings with a higher level of operational properties is relevant. This explains the interest in the use of non-stationary temperature conditions for obtaining protective coatings on structural materials operating in aggressive environments of the by-product coke production. The aggressive conditions of the by-product coke production require the development of new methods for obtaining protective coatings, which make it possible to regulate the composition and structure of protective coatings, to provide the necessary performance characteristics with a short time of their preparation. The coating is a surface layer, purposefully created by the action of the environment on the surface of the part, and characterized by a final thickness, as well as a chemical composition and structural-phase state, qualitatively different from the analogous characteristics of the base material. The insignificant consumption of the coating material and the high characteristics of the surface of the part provide an increased interest in the development of new methods of applying coatings for targeted purposes and the widespread introduction of coatings into industry. Today, the issue of obtaining thicker coatings with a given chemical composition is urgent. An effective (in relation to the substrate) method for improving the surface is chemical-thermal treatment under non-stationary temperature conditions Modeling of temperature fields makes it possible to determine the nature of the propagation of a heat wave caused by the action of an external source, which has time to propagate deep into the substance, and when the surface temperature becomes close to the autoignition temperature , a rather deep heated layer is formed in the substance. This circumstance creates favorable conditions for the development of the reaction, and in the second period there is an intense self-heating due to the chemical reaction of the already heated layers. Temperature time characteristics are important parameters in the preparation of coatings.

Analysis of recent research and publications

The kinetics of the interaction of reagents in waves under unsteady temperature conditions is rather complex and insufficiently studied [1, 2]. The same applies to the kinetics of generation of active atoms in the wave, which will diffuse into the steel. In this work, the kinetics of interaction and heat release in the wave is described with the introduction of the Khaikin-Merzhanov model [3-7]. The Khaikin-Merzhanov model was developed to describe the heterogeneous structure of SHS compositions. This is a model of a reaction cell, which is the closest in terms of thermokinetic and diffuse processes under non-stationary temperature conditions. A reaction center is a region in a sample in which the proportions of each reagent are in a given ratio. A mixture of reagents, capable of synthesis, is a collection of identical reaction cells, which makes it possible to consider any cell as a representative of the entire mixture. To study the heterogeneous structure of the initial compositions, a model was proposed that takes into account the peculiarities of the reaction by recording the kinetic functions in the Arrhenius law

$$D = D_0 \exp\left(-\frac{E_D}{RT}\right),$$

where C — concentration of the diffusing element; E_D — activation energy of its diffusion in steel (or pure iron); D_0 — pre-exponential factor; the values of E_D і D_0 for the diffusion of many elements in α- і γ-Fe are given in the reference literature.

The heterogeneous system is presented in the form of ordered layers of reacting components, as an idealization of real mixed systems and a model of reaction diffusion is introduced. The model assumes that at mutual contact of initial components the new phase is instantly formed is a product AB

separated from initial components A and B. Due to diffusion transfer through a product layer. at the boundaries of the heat is released, resulting in the original components A and B are transferred to the product AB. In [8], we studied the processes in the reaction cell under conditions of self-propagating high-temperature synthesis (SHS) when the sample is heated by an external source at a given law of temperature change from time to time. development of a mathematical model of high-temperature synthesis of nickel aluminide Ni_3A1 for computer modeling and numerical calculations of the main laws governing the synthesis of an intermetallic compound in powder mixtures of nickel with aluminum under conditions of continuous heating of the powder mixture by an external source of energy.

The initial mixture of nickel and aluminum powders was modeled with a set of elementary spherical cells. The unit cell size of the powder system is determined by the dispersion of nickel, the stoichiometry of the composition, and the porosity of the sample. Radius

$$R^3_{\text{e}} = r^3_{\text{Ni}} (1 + \mu_{\text{Al}} \nu_{\text{Al}} \rho_{\text{Ni}} / \mu_{\text{Ni}} \nu_{\text{Ni}} \rho_{\text{Al}}) (1 - h)^{-1},$$

where $\mu_{\text{Al}}, \mu_{\text{Ni}}$ — atomic masses, ν_{Al}, ν_{Ni} — stoichometric coefficients; ρ_{Ni}, ρ_{Al} — density; h — porosity of the mixture.

The number of elementary cells per unit volume

$$N = \frac{1}{4/3\pi R^3_{\text{e}}}.$$

In [9], for modeling the processes of chemical reaction of SHS compositions, an approach was proposed in which the initial heterogeneous composition is modeled by a periodic cellular structure, which is assumed to be homogeneous in thermal and heterogeneous in chemical processes. At the macrolevel, the process of heat transfer is described taking into account the local dynamics of chemical heat release within each unit cell. At the micro level (in the size of a unit cell), the process of mutual diffusion and chemical reaction is modeled.

In [10—13], a mathematical model and the results of a numerical study of the propagation of the combustion front of an SHS composition are presented, when the rate of chemical reaction at each point along the length of the SHS sample is determined from the solution of the problem of diffusion and chemical reaction in reaction cells an averaged element of the heterogeneous structure of a mixture of powders capable of SHS synthesis, containing reacting substances in a proportion equal to their concentration in the mixture. Let us take the form of an element of a heterogeneous structure in the form of a ball, in which there is a substance in the center surrounded by a spherical layer of another substance. In each element of the heterogeneous structure of the SHS composition, the processes of diffusion and reaction of reagents occur at a temperature at the corresponding points of the sample, which changes in time during the reaction. Modeling the processes of formation of protective coatings under non-stationary temperature conditions was carried out for intermetallics, porosity, thermodynamics, during galvanizing, as well as for coatings operating in aggressive conditions of coke production [14—18] made it possible to determine the main factors affecting the technological process of formation of diffusion layers.

Formulation of the study purpose

There are many methods of mathematical modeling of temperature fields. However, at present there is no technique that would completely solve all the problems of detecting temperature features in the process of formation of protective coatings. Therefore, the current direction is the study of models that take into account non-stationary temperature conditions. The purpose of this work is to model the temperature fields obtained during the formation of coatings under non-stationary temperature conditions.

Presenting main material

Since the thermal conductivity depends on the temperature, we use the approximation recommended in [19—21]:

$$G_{i\pm1/2} = \overline{\lambda}\left(\frac{\theta_i^{j+1} + \theta_{i\pm1}^{j+1}}{2}\right) = \overline{\lambda}_{i\pm1/2}, \qquad (3)$$

that is, the dimensionless coefficient of thermal conductivity at half-integer points $i\pm1/2$ is calculated from the arithmetic mean values of temperature at points i and $i\pm1/2$ on the new $(j+1)$-th layer over time.

Numerical calculations are performed in the following order.

First, the kinetic equation (3) is solved. This ordinary differential equation is solved by the Runge-Kutta method of the 4th order of accuracy. Then, after the calculated value $d\eta/dt$ at each point, the initial term F is calculated, which is included in the equation of thermal conductivity and, accordingly, in its divergent form. After that, the numerical solution of the equations of thermal conductivity and diffusion is carried out. The difference equations are nonlinear: the density, heat capacity and thermal conductivity at all points depend on the temperature. Therefore, their linearization is performed: when moving to a new $(j + 1)$-th time layer, these coefficients at all points are calculated using the temperature values on the j-th layer θ_i^j; in particular, value. $\overline{\lambda}_{i\pm1/2}$. Depending on the type of boundary conditions at ($x_1 = 0$) the first pair of run coefficients is calculated: i. Then the forward run is performed: $P_{1½}$ і $R_{1½}$. Then the forward run is performed: the run coefficients at the points $i = 2$,..., N–1. After that, the formulas determine the temperature values on the new, (j + 1)-th layer over time at the point $i = N$ (θ_N^{j+1}).After that, the run back is performed: the value of temperature at all points $(j + 1)$ of the th layer is calculated by the expression: θ_{i-1}^{j+1}, $i = N$–1 ,..., Thus, the developed difference scheme is a scheme of end-to-end calculation.

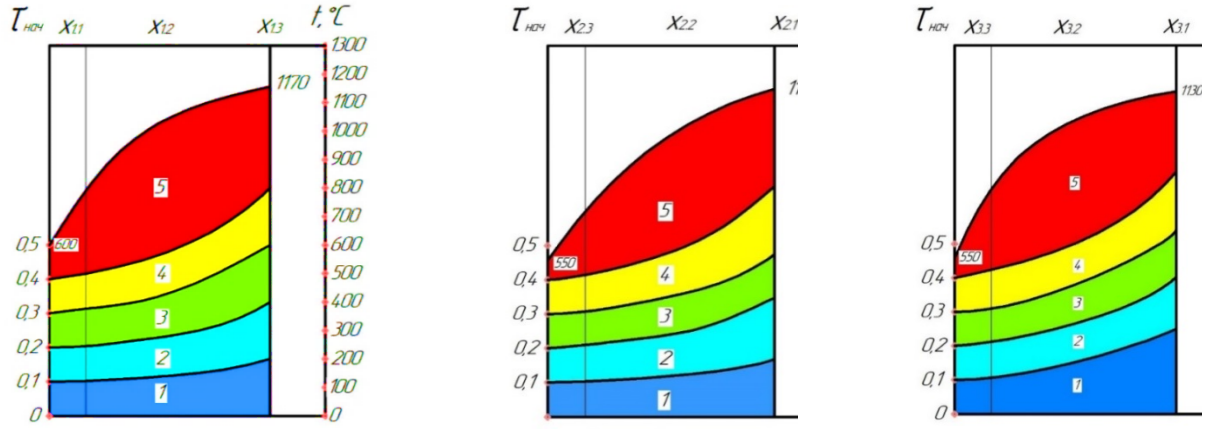
After that, the calculated value θ_{i-1}^{j+1} of the coefficients d_i and $\overline{\lambda}_{i\pm1/2}$ calculated from the calculated values. Then the calculation is repeated, ie iterations are performed. The iteration cycle on this $(j + 1)$-th layer is repeated until the convergence condition is met, when the temperature values and the phase boundary coordinate on two consecutive iterations will differ by a predetermined small value (permissible error):

$$\max_i \left|\theta_i^{j+1,\gamma} - \theta_i^{j+1,\gamma-1}\right| \le \varepsilon_\theta, \quad \max_i \left|\theta_i^{j+1,\gamma} - \theta_i^{j+1,\gamma-1}\right| \le \varepsilon_C, \tag{4}$$

where γ — is the iteration number; $\varepsilon\theta$ — temperature accuracy; εx — the accuracy of the concentration of the diffusing element.

After fulfilling the condition of convergence of iterations, the transition to the next layer in time, and all actions are repeated. The calculations continue until the predetermined maximum time τ_{max} is reached. Since the problem under consideration is two-dimensional, as mentioned above, an intermediate or "half" time layer $\tilde{\tau} = \tau_j + \Delta\tau_j/2$. Initially, the problem of thermal conductivity (or diffusion) is solved on this intermediate layer only along one coordinate axis (for example, along the Ox axis), ie the run back and forth is performed. Then the transition from this "half" layer $\overline{\tau}_{j+1}$ to the "whole" layer $\overline{\tau}_{j+1}$ s carried out and the problem on the second coordinate axis for the axis Oy) — is solved — a run back and forth is performed. When calculating the next "whole" layer over time, the order of alternation of the coordinate axes changes. In this situation, iterations and, accordingly, condition checks (4.59) are performed when calculating each "integer" time layer. To numerically solve the problem, a computer program in Fortran language was developed in the Intel Visual Fortran Composer XE 2011 programming system running in Microsoft Visual Studio 2008. The program consists of a main program that controls the call of subroutines in the required sequence, communicates and data transfer between them, organizes the iteration cycle for numerical solution of the problem, changes the time step with fast or slow convergence of iterations (increase or decrease, respectively), provides display of error messages or the correct completion of the calculation. Subroutines enter the initial data, print the initial data and calculation results when reaching the specified time values, solve the kinetic equation by Runge-Kut method, perform a run back and forth for the thermal and diffusion problem, compare the results of calculations on the current and previous iterations for each layer. time and check the convergence of the iteration under condition (4). The calculated temperature fields at saturation indicate that the whole process can be divided into two stages: by heating time τnagr = 0,5 h. at A = 1,5 B = 4, when the wave passes from the walls of the container X13, X23, X33 (T1) everywhere

charge X12, X22, X32 (T2) to the surface of the part X13, X21, X31 (T3). The plane of the temperature field (in case of spontaneous combustion-5) increases depending on the autoignition temperature and the maximum temperature. Thus, a number of increases in the temperature field are formed depending on the saturating element during: titanization - vanadiuming - alliteration. The overall picture is most affected by the maximum temperature (1130 °C - 1150 °C - 1170 °C) and the speed of propagation of the autoignition wave, which is represented by fields 1—4.



а – alliteration б – vanadiuming в – titanization

Fig. 1. Estimated values of the temperature field for different types of coverage (1—4 heating zones, 5 — thermal spontaneous combustion zone, A = 1,5 V = 4)

Conclusions

The temperature fields at saturation in non-stationary temperature conditions are determined in the work, which allowed to establish two zones: the heating zone and the zone of thermal spontaneous combustion. Modeling of temperature fields obtained during the formation of coatings under nonstationary temperature conditions is considered. In this paper, the kinetics of interaction and heat release in a wave is described using the Haikin-Merzhanov model. This is a model of the reaction cell, which is closest in thermokinetic and diffusion processes under non-stationary temperature conditions. The plane of the temperature field increases depending on the autoignition temperature and the maximum temperature. The series of growth of the temperature field depending on the saturating element is as follows: titanation - vanadium - alliteration. The maximum temperature (1130 °C - 1150 °C - 1170 °C) and the speed of propagation of the autoignition wave have the greatest influence on the general picture.

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МОДЕЛЮВАННЯ ТЕМПЕРАТУРНИХ ПОЛІВ ОТРИМУВАНИХ ПРИ ФОРМУВАННЯ ПОКРИТТІВ ПРИ НЕСТАЦІОНАРНИХ ТЕМПЕРАТУРНИХ УМОВ

Середа Б.П., Хина Б.Б., Кругляк І.В, Середа Д.Б.

Реферат

Розглянуто моделювання температурних полів одержуваних при формуванні покриттів при нестаціонарних температурних умовах. В роботі кінетика взаємодії і тепловиділення в хвилі описується з використанням моделі Хайкіна-Мержанова. Модель Хайкіна-Мержанова розроблена для опису гетерогенної структури СВС складів. Це модель реакційної комірки, яка найбільш близька по термокінетичним та дифузійним процесам при нестаціонарних температурних умовах. Чисельні розрахунки проводяться в наступному порядку.

Спочатку вирішується кінетичне рівняння методом Рунге-Кутта 4-го порядку точності. Потім після розрахованого значенню $d\eta/dt$ в кожній точці обчислюється початковий член F, який входить до рівняння теплопровідності і, відповідно, в його дивергентну форму. Після цього здійснюється чисельне рішення рівнянь теплопровідності та дифузії. Різницеві рівняння є нелінійними: щільність, теплоємність та коефіцієнт теплопровідності у всіх точках залежать від температури. Тому виконується їх лінеаризація: при переході на новий (j + 1)-й часовий шар ці коефіцієнти у всіх точках розраховуються, використовуючи значення температури на j-му шарі θ_i^j; зокрема, значення $\overline{\lambda}_{i\pm1/2}$. В залежності від типу граничних умов при $x_1 = 0$) обчислюється перша пара прогоночних коефіцієнтів: $P_{1½}$ і $R_{1½}$. Потім виконується прогін вперед: обчислюються прогоночні коефіцієнти в точках i = 2 ,..., N–1.Після цього за формулами визначаються значення температури на новому, (j + 1)-му шарі за часом в точці i = N (θ_N^{j+1}). Після цього виконується прогін назад: за виразом обчислюються значення температури у всіх точках (j + 1)-ого шару: θ_{i-1}^{j+1}, i = N–1 ,..., 2. Таким чином, розроблена різницева схема є схемою наскрізного розрахунку. Розрахункові температурні поля при насиченні свідчать, що увесь процес можливо розбити на дві стадії: за часом нагрівання $\tau_{нагр}$ = 0,5 год. при A = 1,5 B = 4, коли хвиля проходить від стінок контейнера X13, X23, X33 (T1) скрізь шихту X12, X22, X32 (T2) до поверхні деталі X13, X21, X31 (T3). Площина температурного поля (при самозайманні — 5) збільшується в залежності від температури самозаймання та максимальної температури.

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