

ЛІТЕРАТУРА

1. Benavides-Prada O., Guevara-Lastre C., Barón-Núñez F., Barajas-Ferreira C., Ortiz-Basurto R., Torrestiana-Sánchez B. & Muvdi-Nova C. Vacuum membrane distillation: Modeling and analysis for recovery of ethanol from ethanol/water solutions. *CT&F - Ciencia, Tecnología y Futuro*. 2013. Vol. 5. No. 2. P. 47–60.
2. Ладієва Л. Р., Жулинський О. А. Математична модель процесу контактної мембранної дистиляції. *Автоматика. Автоматизація. Електротехнічні комплекси і системи*. 2004. №2. С. 46–51.
3. Ладієва Л. Р., Жулинський О. А. Математична модель процесу контактної мембранної дистиляції. *Автоматизація виробничих процесів*. 2005. №1. С. 19–21.
4. Ладієва Л. Р., Оніщенко В. О., Дубік Р. М. Математичне моделювання розподілу температур у мембранному модулі в процесі мембранної дистиляції. *Наукоємні технології*. 2015. № 1. С. 5–8.

SIMULATION OF THE THERMOKINETICS OF REACTIVE SINTERING OF NICKEL WITH ALUMINUM IN THE INTERVAL OF EUTECTIC DECOMPOSITION OF INTERMETALLIDE

Solntsev V. P.¹, Shakhnovsky A. M.², Kvitka O. O.², Petrash K. M.¹, Solntseva T. A.¹, Terekh T. Yu.²

МОДЕЛЮВАННЯ ТЕРМОКІНЕТИКИ РЕАКЦІЙНОГО СПІКАННЯ НІКЕЛЮ З АЛЮМІНІЄМ В ІНТЕРВАЛІ КОНЦЕНТРАЦІЙ ЕВТЕКТИЧНОГО РОЗПАДУ ІНТЕРМЕТАЛІДУ

Солнцев В. П.¹, Шахновський А. М.², Квітка О. О.², Петраш К. М.¹, Солнцева Т. А.¹, Терех Т. Ю.²

МОДЕЛИРОВАНИЕ ТЕРМОКИНЕТИКИ РЕАКЦИОННОГО СПЕКАНИЯ НИКЕЛЯ С АЛЮМИНИЕМ В ИНТЕРВАЛЕ КОНЦЕНТРАЦИЙ ЭВТЕКТИЧЕСКОГО РАСПАДА ИНТЕРМЕТАЛЛИДОВ

Солнцев В. П.¹, Шахновский А. М.², Квитка А. А.², Петраш К. Н.¹, Солнцева Т. А.¹, Терех Т. Ю.²

¹Інститут проблем матеріалознавства ім. І. М. Францевича НАН України
Київ, Україна
solntcevvp@gmail.com

²Київський політехнічний інститут імені Ігоря Сікорського
amshakhn@xtf.kpi.ua

On the basis of the proposed thermokinetic model, the thermal behavior of the reaction system of nickel with aluminum during sintering has been studied. A computer experiment has been used to study the influence of the temperature of the external environment, as well as the temperature of initiation on the nature of the ongoing processes. It has been established that the optimal for reaction sintering is to ensure the proximity in terms of the initiation temperature and the external environment.

Key words: reaction sintering, nickel, aluminum, thermokinetic model, initiation temperature, radiation

На основі запропонованої термокінетичної моделі вивчено теплову поведінку реакційної системи нікелю з алюмінієм під час спікання. Із використанням комп'ютерного експерименту досліджено вплив температур зовнішнього середовища, температурного ініціювання на характер процесів, що протікають у системі. Встановлено, що оптимальним для реакційної спікання є забезпечення близькості за величиною температур ініціювання та зовнішнього середовища.

Ключові слова: реакційне спікання, нікель, алюміній, термокінетична модель, ініціація температура ініціювання, випромінення

На основе предложенной термокинетической модели изучено тепловое поведение реакционной системы никеля с алюминием при спекании. Компьютерным экспериментом исследовано влияние температуры внешней среды, температуры иницирования на характер протекающих процессов. Установлено, что оптимальным для реакционного спекания является обеспечение близости по величине температур иницирования и внешней среды

Ключевые слова: реакционное спекание, никель, алюминий, термокинетическая модель, температура иницирования, излучение

INTRODUCTION

The most important thing in creating a new generation of heat-resistant powder materials is to ensure high plastic properties of alloys (both technological and mechanical). This is especially true for the production of dispersion-hardened materials, when liquid-phase methods cannot be used in the technology of their production.

Fedorchenko and Pugina [1], as well as Kostetskiy B. et al. [2] hypothesized the emergence of the so-called "third body". In accordance with this hypothesis, an intermediate layer appears between the rubbing surfaces of solids with physicochemical and mechanical properties that differ from the bulk of the contacting materials. This assumption has been experimentally confirmed by a large number of studies carried out mainly in the study of the mechanisms of friction and wear of materials. However, in his early works on iron sintering, authors [1] also had in mind solid-phase sintering, in which a special state arises in the intercrystalline space, leading to a loss of plasticity and other physical and mechanical properties of the material.

The use of reaction sintering in the preparation of dispersion-hardened nickel alloys allowed the authors of this work to obtain materials with a high level of technological plasticity, impact toughness, and fatigue strength [3]. Such properties are evidently associated the peculiarities of the process, in particular, the high rate of the reaction interaction of nickel with aluminum, which was experimentally established in the study of the thermokinetics of the processes [4]. In this case, sintering occurs at the same rate and the reaction crystallization of the intermetallic compound, which prevents the coagulation of dispersed particles of an inert hardener (for example, yttrium oxide or other compounds).

Scientific interest in the processes of synthesis and sintering of compositions with the participation of exothermic reactions is caused in connection with the practical problems of using a large amount of free energy for the consolidation of materials, and also has an important fundamental aspect in connection with the study of collective processes that determine the evolution of nonequilibrium physicochemical systems and form the structure

and properties of composite materials [5]. As a rule, the released heat of an irreversible reaction process significantly exceeds the accumulated free surface energy of the powder system. However, the released chemical energy, in contrast to the free energy of a powder body, does not lead to consolidation of the system, but to an increase in porosity, and sometimes to destruction. This behavior is due to the high rate of synthesis reactions in which, along with the high rate of release of thermal energy, reaction crystallization of compounds is observed, which apparently leads to an increase in pressure in the reaction liquid and accelerated formation of large pores and cavities from small pores formed during unipolar dissolving a eutectic or peritectic liquid of one of the refractory components.

It was experimentally established earlier [6] that the volumetric changes in the billets of composite materials during reaction sintering depend on the thermokinetic trajectory of the process. In the absence of an explosive change in the temperature of the sample or in the case of the oscillatory behavior of the reaction system, sintering and shrinkage of the composition is observed. Previously, the thermal behavior of the system was investigated depending on some kinetic parameters [7], the values of which determine the required behavior of the system. Equally important and is of not only theoretical but also practical interest for determining such conditions is external temperature at which the reaction system is located as well as the temperature of the initiation of the process.

RESEARCH METHODS

For the first time, in contrast to the formal phenomenological approach developed in the works of A. Merzhanov [8], a physicochemical thermokinetic model of synthesis was proposed [9], based on the synergistic principle of description, where the reaction liquid is considered as a flow reactor. The most significant results of the development of this model were obtained in [10, 11]. In these works, the thermokinetics of the synthesis of compounds was directly modeled. The mathematical description of the processes observed in such systems is presented by a thermokinetic model of the synthesis of a compound with a hidden maximum. As the result was the establishment of the multivariance of the evolution of irreversible processes in the synthesis of specific compounds and the establishment of safe modes of its implementation in a variety of control parameters and external conditions. In reaction sintering, despite the general approach to the construction of the model, it is necessary to take into account the final result and consider the equilibrium state as an attractor to which the reaction powder system tends. However, it is necessary to establish the conditions and parameters under which the system selects the required thermokinetic trajectory that provides the required macroscopic behavior, for example, shrinkage or dispersion of the structure of the reaction billet.

In this context, the system is considered as a flow-through reactor of ideal mixing. In this case, we consider the region where, in addition to the synthesis of the intermetallic compound, which is observed above the melting point of aluminum and its decomposition occurs at temperatures in a given concentration region.

Thus, the mathematical model can be represented by the system:

$$\left\{ \begin{array}{l} \frac{dX}{dt} = k_1(1-X) - k_2XY - k_3\frac{X}{T} + k_4(T-1385) \\ \frac{dY}{dt} = -k_2XY + k_4(T-1385) \\ C\frac{dT}{dt} = k_1(1-X)H_1 + k_2XYH_2 + k_3\frac{X}{T}H_1 - k_4(T-1385)H_2 - \\ -l(T-T_a) - \varepsilon\sigma T^4 + \varepsilon\sigma T_a^4 \end{array} \right. \quad (1)$$

where X , Y are concentrations of soluble refractory components in the melt; k_1 is dissolution rate constant, k_2 is intermetallic compound formation reaction rate constant NiAl; k_3 is melt crystallization rate constant; k_4 is intermetallic decomposition rate constant; T is current temperature of the Ni-Al system; T_a is temperature of the external environment, C is system heat capacity; h_1 is heat of dissolution of nickel in aluminum; l is specific crystallization constant; ε is the degree of blackness (note, that in this study $\varepsilon=1$ that of a completely black body); σ is the Stefan-Boltzmann constant; H_1 is heat of formation of NiAl intermetallic compound; H_2 is heat of complex decomposition of NiAl intermetallic with the formation of Ni₃Al and Ni according to the state diagram.

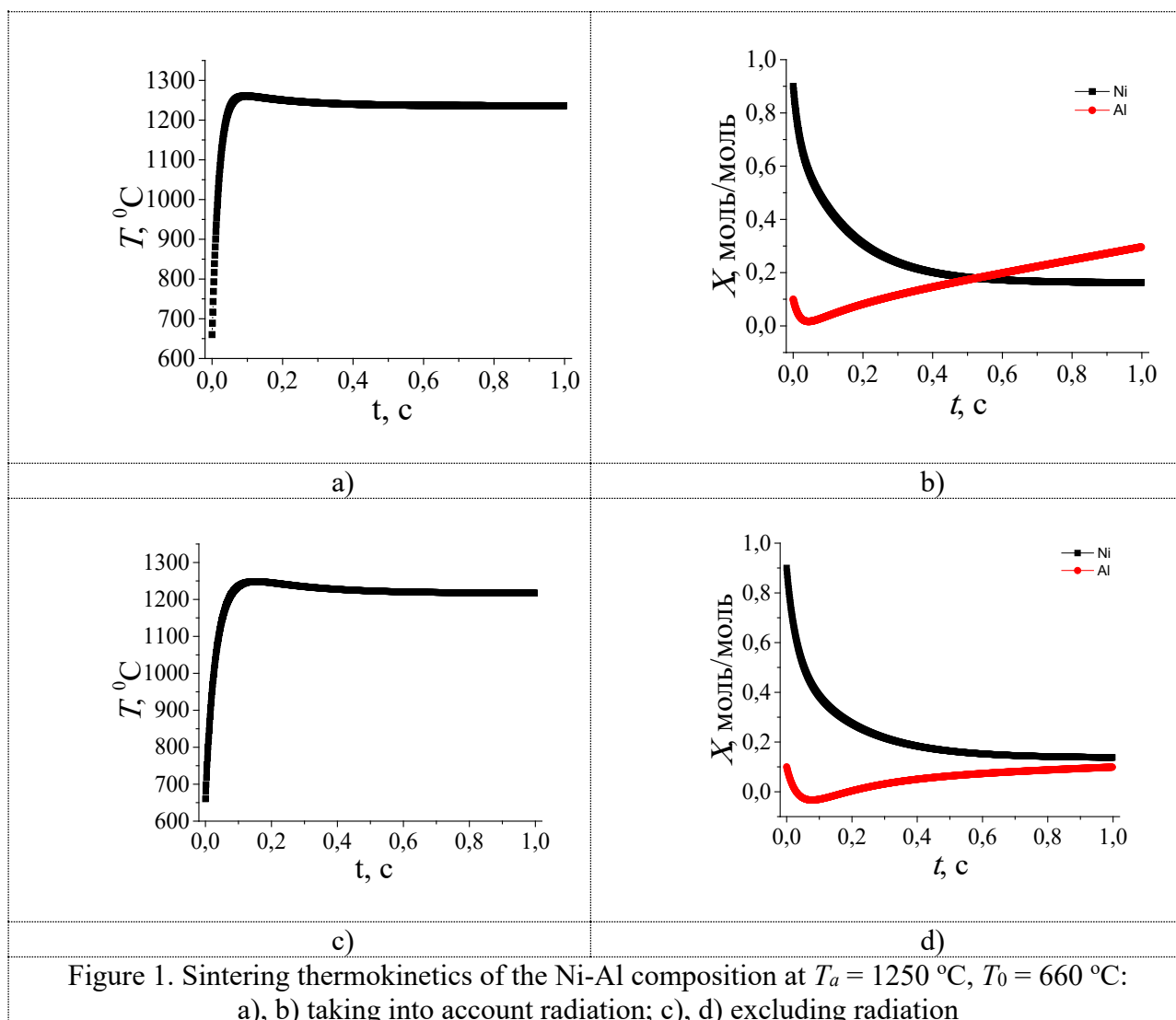
The first and second equations of the system (1) represent the material balance, and the third equation represents the heat balance. It is assumed that heat transfer between the system and the environment occurs according to the Newtonian mechanism, as well as radiation. The first and fourth terms of the equations describe the processes of the entry of the refractory component into the system by means of its dissolution and decomposition of the intermetallic compound, respectively, and the second and third withdrawal thereof due to the reaction of synthesis and crystallization. The second term is associated with the escape of components due to a chemical reaction, and the third is due to the crystallization of the refractory nickel component.

RESULTS AND DISCUSSION

The thermokinetics of the sintering process was studied at the following identical values of the following parameters: $k_1 = 1$; $k_2 = 1$; $k_3 = 1000$; $k_4 = 0,01$.

The solution of the mathematical model was carried out by the Euler method using a program developed in the Visual Basic 6.0 environment.

It is possible to exclude the influence of the thermal radiation factor from the calculations at any possible values of the parameters in the software, while obtaining a new theoretical curve of the temperature change as a function of time (in the time interval from 0 to 100 seconds). It is noted that the indicated time interval is quite sufficient for studying the thermokinetic trajectory, since the overwhelming majority of the studied reaction processes proceed much faster and come to a stationary state much earlier than the maximum specified in the program.



Presented work evaluated the influence of two technological factors, namely the ambient temperature, i.e., heating device (furnace), and the temperature of initiation of the reaction of interaction of nickel with aluminum, at the given values of the control parameters, the rate constants of the processes.

Upon slow heating to the melting point of aluminum, the initiation temperature coincides with the melting point. However, in this study, the authors were interested in the accelerated version of sintering, in which the sintered sample is placed in a heated furnace. In this case, the initiation temperature depends on random factors and will be in the range of aluminum melting temperatures and furnace temperatures.

Thermokinetic patterns (Figure 1, Figure 2 and Figure 3) were calculated according to the data [12]. In the case of initiation of the reaction at the melting temperature of aluminum (Figure 1), a sharp uncompensated rise in temperature is observed, since the mechanisms of energy dissipation are not activated. However, when the maximum temperatures are reached, the processes of decomposition of the intermetallic compound and heat removal into the external environment are activated. As a result, the temperature becomes almost constant. At the same time, it is necessary to take into account the behavior of the system at the stage of temperature rise; in this time domain, stresses arise, the growth

of cavities, which leads to the appearance of material defects and the loss of its functional properties.

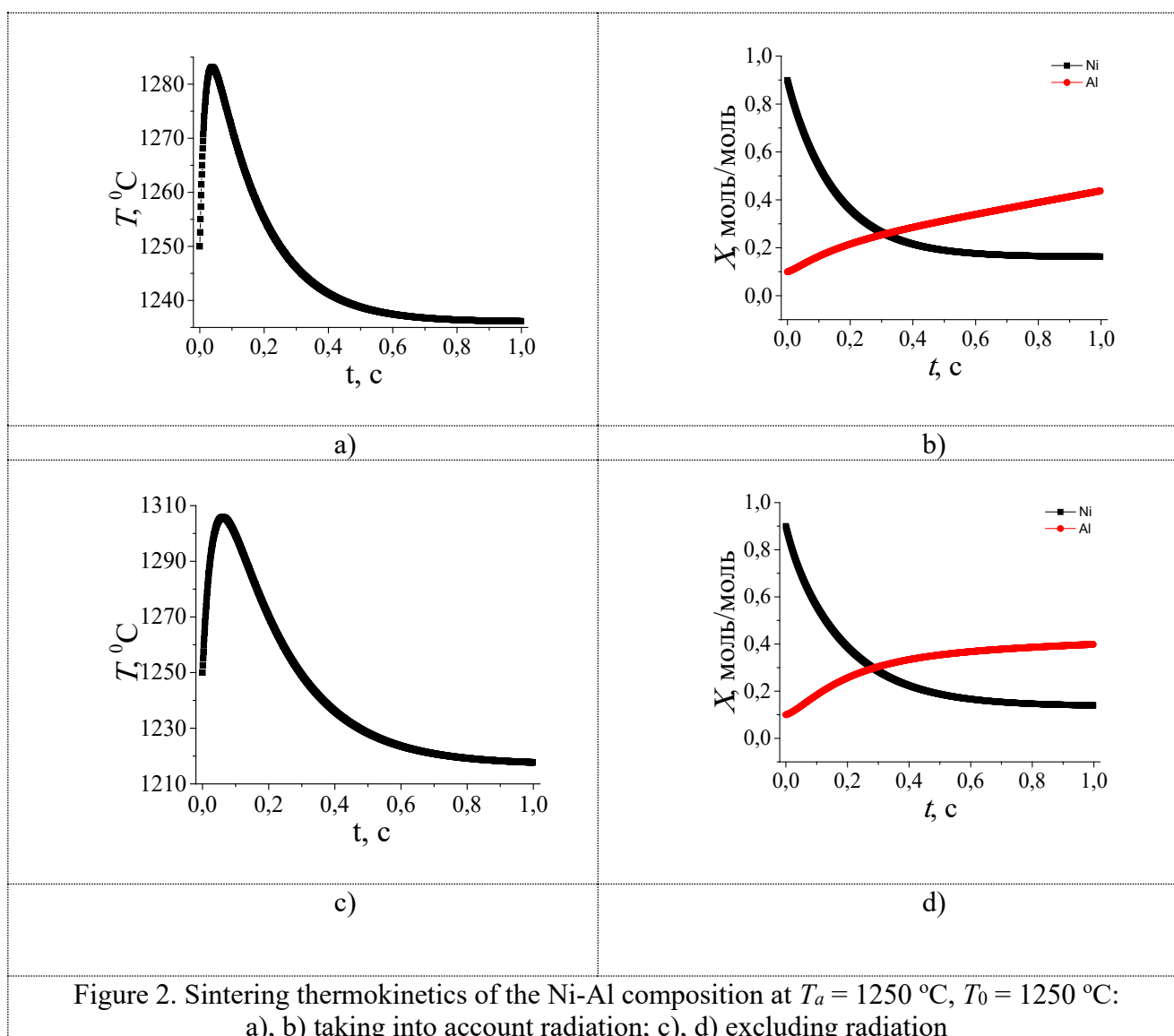


Figure 2. Sintering thermokinetics of the Ni-Al composition at $T_a = 1250\text{ }^{\circ}\text{C}$, $T_0 = 1250\text{ }^{\circ}\text{C}$: a), b) taking into account radiation; c), d) excluding radiation

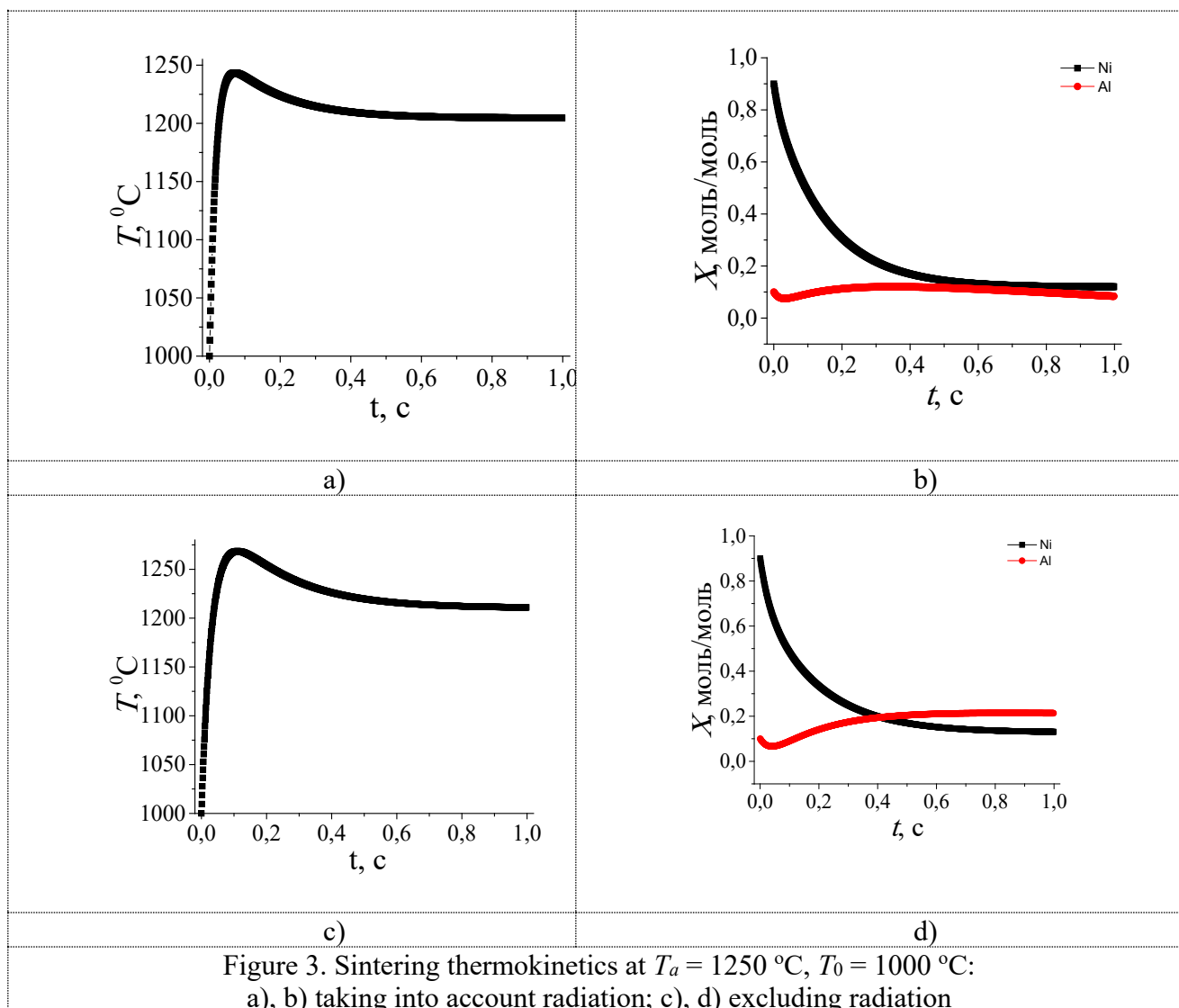
Of particular interest is the case when the ambient temperature is equal (or is close) to the initiation temperature. In this case (Figure 2), the temperature spike is about $50\text{ }^{\circ}\text{C}$. Naturally, with such heating temperature gradients, the probability of the formation of macrodefects in the material structure is minimal. Therefore, when sintering the reaction compositions, it is necessary to ensure the heating of the material billets to the ambient temperature in a time less than the latency period.

As can be seen from Figures 2 and 3, the rate of temperature rise depends on the temperature difference between the external environment and the initiation temperature. Thus, the most favorable sintering mode is the closeness of the ambient temperature to the initiation temperature.

CONCLUSIONS

The thermokinetic behavior of the system was calculated on the basis of a model describing the processes of reaction sintering. The optimum temperatures for the initiation of the reaction of the interaction of aluminum with nickel and the thermal state of the

external environment have been determined. In this case, the temperature of the external environment in the case of energy transfer by radiation can be controlled by the process of reaction sintering. In the prospect of further research is the study of the influence of the members of the model, related to crystallization of the refractory nickel component, on the stiffness of the model.



REFERENCES

1. Федорченко И. М., Пугина Л. С. Композиционные спеченные материалы. Киев: Наукова думка, 1980. 404 с.
2. Носовский И. Г., Исаев Э. В., Костецкий Б. И. О роли кристаллического строения при трении и схватывании металлов. *Докл. АН СССР*. 1971. Т.198, №1. С. 78–82.
3. Солнцев В. П. и др. Разработка дисперсно-упрочненного порошкового сплава на основе нихрома и технологии изготовления из него макета металлической теплозащитной конструкции. *Порошковая металлургия*, №11/12. Київ. 2018. С. 23–32.
4. Солнцев В. П. и др. Термокинетика реакционных процессов, инициированных контактным плавлением в порошковых металлических смесях на основе никеля с алюминием. *Сборник научных трудов «Адгезия расплавов и пайка материалов»*, вып. 47. Киев. 2014. С. 25–34.

5. Солнцев В. П. и др. О механизме спонтанного возникновения пространственно-временной организованной структуры в порошковых реагирующих системах при контактном плавлении компонентов. *Доп. НАНУ*. 2010. №3. С. 105–111.
6. Солнцев В. П., Скороход В. В., Солнцева Т. А. Коллективные процессы при реакционном спекании с участием жидкой фазы. *Порошковая металлургия*. 2010. №3/4. С. 22–29.
7. Solntsev V. P et al. Simulation of thermokinetics of the reactive sintering process in a powder nickel-aluminum mixture. *Комп'ютерне моделювання в хімії та технологіях і системах сталого розвитку – КМХТ-2020: Збірник наукових статей Восьмої міжнар. наук. – практ. конф. Київ, КПІ ім. Ігоря Сікорського, 2020. С.126–132.*
8. Мержанов А. Г. Новые модели горения второго рода. *ДАН СССР*. 1977. Т.223. №6. С. 1130–1133.
9. Солнцев В. П. и др. Развитие физико-химических представлений о природе СВС на основе синергетического подхода. *Прикладная синергетика, фракталы и компьютерное моделирование структур*. Томск: ТГУ. 2002. С. 163–168.
10. Петраш К. Н., Солнцев В. П., Солнцева Т. А. Влияние характера переноса тепла на термокинетические траектории процессов синтеза интерметаллидов NiAl₃ и Ni₃Al. *Математические модели и вычислительный эксперимент в материаловедении*. вып. 20. Киев. 2018. С. 110–114.
11. Петраш К. Н. и др. Роль переноса тепла излучением в высокотемпературных реакционных процессах синтеза интерметаллида NiAl. *Порошковая металлургия*. №7/8. Киев. 2017. С. 39–46.
12. Zhang Ch.-H. et al. Chen's lattice inversion embedded-atom method for Ni-Al alloy. *Chinese Physics Bul.* 2012. Vol. 21. No. 11. P. 113401-1–113401-7. DOI: 10.1088/1674-1056/21/11/113401

ДОСЛІДЖЕННЯ ПРОЦЕСУ ІОННОГО ОБМІНУ ШЛЯХОМ СТАТИСТИЧНОГО АНАЛІЗУ ВИРОБНИЧИХ ДАНИХ

Мердух С. Л.

ИССЛЕДОВАНИЕ ПРОЦЕССА ИОННОГО ОБМЕНА ПУТЕМ СТАТИСТИЧЕСКОГО АНАЛИЗА ПРОИЗВОДСТВЕННЫХ ДАННЫХ

Мердух С. Л.

INVESTIGATION OF THE ION EXCHANGE PROCESS BY STATISTICAL ANALYSIS OF PRODUCTION DATA

Merdukh S. L.

Національний технічний університет України
«Київський політехнічний інститут імені Ігоря Сікорського»

Київ, Україна

merdukh.svetlana@gmail.com