UDC 544.3:669.71

Yu. Belokon′ doctoral candidate, c.t.s.
J. Oginskiy, head. of department, d.t.s.
K. Belokon′, associate professor, c.t.s.
A. Zherebtsov, senior teacher

THEORETICAL AND EXPERIMENTAL DETERMINATION OF ENERGY OF ACTIVATION FOR FORMATION OF INTERMETALLIDES IN SYSTEMS «NICKEL-ALUMINIUM» AND «TITAN-ALUMINIUM»

Zaporizhska state engineering academy

Two methods of determination of activation energy for reaction of formation of intermetallides are considered: theoretical method of calculation which is based on the results of thermodynamics analysis of flowing of SHS-reactions, and experimental method, based on research of kinetics of formation of intermetallide phases. It is set that activation energies for the systems Ni-Al and Ti-Al fold ~45 and ~82 kJou/mole respectively. It is shown that a difference between the values of activation energies, got noted methods, does not exceed 5 %. Got results can be applied for the further calculations of physical and chemical model of flowing of reactions for the intermetallide systems at non-stationary temperature conditions.

Keywords: activation energy, SHS-reaction, thermodynamics analysis, kinetics, intermetallides

Entry. During the estimation of possibilities of making of different inorganic connections, including. intermetallide, a kinetic and thermodynamics analysis acquires of greater value the method of self- high temperature synthesis (CBC), first of all through determination of activation energy for formation of intermetallide at non-stationary temperature conditions [1].

It is known that SHS-processes are based on the use of warmth which is distinguished during the stronglyexotermic reaction of co-operation of powder-like reagents. For the real conditions, when the charges of warmth do not equal a zero, it is necessary for stationary distribution of wave of burning, that speed of reaction and, thus speed of calorification is in a reactionary area, were far anymore than speed of heat emission to the environment. Except for that, speed of reaction must substantially increase with the increase of temperature which is characterized by energy of activation of reaction [2]. Therefore activation energy (E_a) - energy, which is needed for achievement of the system by transitional state, called the activated (or transitional) complex which grows into products of reaction wilfully. Than less is activation energy of reaction, the higher speed of its flowing.

Lately the far of works are appeared [3-6], where results over of research of high temperature synthesis of intermetallide alloys at SHS-conditions are brought. In these most works, sacred to the synthesis of the intermetallide systems on the mode of heat explosion, the special attention is spared to composition, to the structure and properties of the got products. However variation of experimental data from activation energy of SHS-process, and also the very wide range of values date, that different authors point, does comparison not enough convincing. So, in works [1,2] on the basis of thermodynamics analysis a value ΔH_T, ΔG_T is set in the interval of

temperature 298-1400 K for chemical compounds which appear in the double systems on the basis of aluminium (*Ni-Al* and *Ti-Al*). Thus, the got dependences allow to estimate effective or imaginary activation energy of reaction for formation of intermetallide.

Raising of task. The purpose of work consists in determination of activation energy of reaction a theoretical and experimental way in the intermetallide systems of *Ni-Al* and *Ti-Al*, that will allow to expect critical conditions and period of induction of these reactions.

Main part of researches. Two methods of determination of activation energy of reaction for formation of intermetallide are examined: theoretical method of calculation with the use of results of thermodynamics analysis of flowing SHS-reactions, and also experimental, based on research of kinetics of formation of intermetallide phases.

It is set on the basis of the executed thermodynamics calculation, that the reaction of formation of intermetallide connections flows in direct direction at all possible temperatures of carry out of process. The large values of constant of equilibrium (for example, for *TiAl*: $k = 2{,}3 \cdot 10^{11}$) shows, that at the standard conditions of equilibrium a reaction is considerably displaced on the right, and it means that at temperature 298 K appears proof connections of intermetallides. At temperatures which are less 933 K a reaction flows very intensively, what the very high value of constant of reaction testifies.

The values of activation energy of reaction for formation of intermetallide alloys fold: $E_a(_{NiAl})$ = 45.153 kJou/mole; $E_a(_{TiAl})$ = 82.263 kJou/mole.

For confirmation of results of theoretical calculations experimental researches of kinetics of co-operation of intermetallide alloys of the systems *Ni* were executed - *Al* and *Ti-Al* at the conditions of SHS, with the further making of analytical equations of temperature-temporal dependences.

For research of processes of co-operation of nickel and aluminium in the hard state samples annealed at temperatures from 300 to 500 °C through every 10 °C with even time of self-control (~5 min.). In the system *Ni-Al* look a clear latent period duration of which diminishes with the increase of temperature [3,4]. By research of structure of samples of Ni-*Al* depending on a temperature and time of heating the moment of appearance of intermetallide determined size (0.5-1.0 mcm) is fixed at each of investigational temperatures. The got great number of empiric values we were added to approximation by method least-squares procedures to exponential equation. By means of application package for the engineer-mathematical calculations of «*SciLab*» the calculation values of energy of activation and pre-exponential index were found.

Calculation of activation energy for formation of the first intermetallide crystals on experimental results for connection of *NiAl* is evened ~43 kJou/mole, and for connection of *TiAl* presents ~79 kJou/mole.

Conclusions.

1. For determination of activation reactions the theoretical method of thermodynamics to the analysis and experimental from the study of kinetics of formation of intermetallide phases was considered.

2. It is set that the results of experimental researches confirm theoretical calculations: a relative error does not exceed 5 %.

REFERENCE

1. **Бєлоконь, Ю. О.** Термодинамічний аналіз протікання СВС-реакцій у системі «нікель-алюміній» [Текст] / Ю. О. Бєлоконь, О. В. Харченко, К. В. Бєлоконь, С. В. Башлій Металургія : наукові праці Запорізької державної інженерної академії. – Запоріжжя : РВВ ЗДІА, 2016. – Вип. 1 (35). – С. 43-47.
2. **Бєлоконь, Ю. О.** Термодинамічний аналіз протікання СВС-реакцій у системі «титан-алюміній» [Текст] / Ю. О. Бєлоконь // Металургія : наукові праці Запорізької державної інженерної академії. – Запоріжжя : РВВ ЗДІА, 2016.– Вип.. 2 (36). – С. 66-71.
3. **Sereda, B.** The Researching and Modeling of Physical-Chemical Properties of Ni-base Alloys in SHS Conditions [Text] / B. Sereda, Yu. Belokon', A. Zherebtsov, D. Sereda // Materials Science and Technology. – 2012. – Vol. – Pp. 494-498.
4. **Середа, Б. П.** Исследование влияния фазового состава Ni-Al сплавов на физико-химические свойства скелетных никелевых катализаторов [Текст] / Б. П. Середа, Г. Б. Кожемякин, К. В. Савела и др. // Металургія : наукові праці Запорізької державної інженерної академії. – Запоріжжя : РВВ ЗДІА, 2009. – Вип. 20. – С. 112-117.