INFLUENCE OF TEMPERATURE OF INITIATION AND ENVIRONMENT IN SHS ON THE TERMOKINETICS BEHAVIOR OF REACTING SYSTEM

V.P.Solntsev[1], A.M.Shakhnovsky[2], V.V.Skorokhod[1], K.N.Petrash[1,2]
[1] Frantsevich Institute for Problems of Materials Science NAS Ukraine, Kiev, Ukraine
[2] National Technical University of Ukraine "KPI", Kiev, Ukraine
3, Krzhyzhanovsky Str., Kiev, 03680, Ukraine, e-mail: SolntcevVP@gmail.com

Thermokinetic model of the synthesis of compound with hidden maximum was proposed earlier [1]. In this work, the refined model appears to account for the dependence of the equilibrium concentration of the reaction components on the temperature. Thermokinetic model to account for this is given by

$$\dot{X} = k_1[a(T) - X] - k_2 X - k_3 \frac{l}{h}(T - T_a),$$

$$C\dot{T} = -k_1(a - X)h + k_2 XH + g - l(T - T_a)$$

where X - the concentration of the solvent component in the liquid melt, $a(T)$- its equilibrium concentration in the melt k_1 and k_2 - rate constants of dissolution and fusion reaction , h - enthalpy of dissolution of the solid component in the melt or its crystallization from the melt and H - enthalpy of fusion reactions, C - heat capacity, l- heat-transfer coefficient, T - temperature, T_a - ambient temperature. Function of the equilibrium concentration $a(T)$ was determined on the basis of experimental data of the equilibrium phase diagram of the titanium-aluminum [2].

As an approximating function is most advisable to take a logarithmic function of the next form:

a(T) = 99944,758 – 44426,468 ln(T) + 6588,649 ln(T)^2 – 325,684 ln(T)^3.

Termokinetics behavior has been studied in a variety of control parameters: the reaction initiation temperature synthesis, the ambient temperature and the rate constants of dissolution. The results of computer simulation show multivariant thermokinetic behavior (Fig. 1.2). However, first of all we pay attention to the result, indicating one of the mechanisms of thermal explosion, which has an evident synergistic nature. The results given in Figure 2, clearly show a greater degree of role of the initiation temperature and environment.

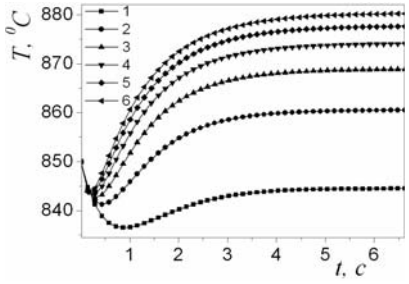

Fig.1 Thermokinetics of reacting of aluminum with titanium at temperatures of 850 ^{0}C and initiating an environment at 800^{0}C in k_1 = 1, 2, …6 and k_2=1

In this regard, the development of synthesis technology needs identifying some areas in a set of control parameters, excluding thermal explosion.

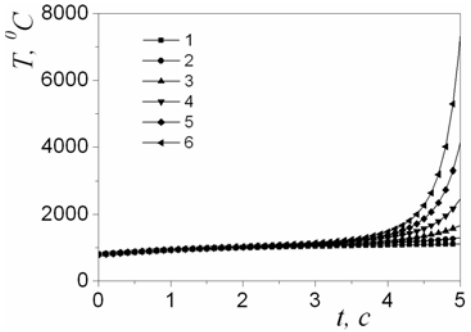

Fig. 2 Thermokinetics of reacting of aluminum with titanium at temperatures of 800^{0}C and initiating an environment at 1000^{0}C in k_1 = 1, 2, …6 and k_2=1

1.Солнцев В.П., Скороход В.В. Термокинетическая модель и механизм реакционного взаимодействия, инициированного перитектическим плавлением // Доп. НАНУ- 2009 - №11 - С. 91-97.
2. Корнилов И.И. Титан. Источники, составы, свойства, металлохимия и применение. - М.:Наука, 1975. - 310 с.