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A closer look at the computer modeling and sintering optimization in the preparation of YAG

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Abstract   Recently, we presented a method for estimation of the diffusion and reaction rates of synthesis at high temperatures using limited information, such as synthesis time and dimensions of reactants, from real laboratory experiments (Mackevičius et al. in Central Eur J Chem 10(2):380–385, 2012). There, we restricted ourselves to the one- and two-dimensional models. Having both adapted our computing program to the three-dimensional case and significantly speeded it up, now we are able present the results in the three-dimensional model. Solving an inverse modeling problem, we obtain explicit formulas for the diffusion coefficient and reaction rate as functions of temperature. We calculate the activation energies and other parameters, thus obtaining conditions for occurrence of synthesis. In addition, using the results of the three-dimensional model, we find the optimal temperature for energy consumption in the YAG synthesis.

Keywords   Sol–gel and solid-state reactions · Diffusion coefficient · Reaction rate · Occurrence of synthesis · Activation energy · Energy consumption optimization

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1 Introduction

The rate of a general homogeneous reaction is conventionally measured by following the decrease in concentration of reactants or the increase in concentration of the products at constant temperature. For the heterogenous reaction, however, the concept of concentration no longer has the same significance, and the progress of reaction is usually determined in some other way. The kinetics and the mechanism studies of heterogeneous reactions thus involve measurement of changes in mass of reactants of the sample as functions of time at constant temperatures [2–5]. Many equations relating the rate of solid-state reactions under isothermal and nonisothermal conditions to the bulk nucleation followed by three-dimensional growth and diffused distribution at the phase boundary (classical Fick diffusion or Prout–Tompkins model) are summarized and discussed in the literature [6–10]. The interpretation of the kinetic equations is extremely complicated and considers the way in which the reaction starts, by a process of nucleation, then how those nuclei grow and what reaction or interface geometry is involved, and finally, how the reactants decay. Consequently, for the investigation of complex solid-state reactions different novel mathematical approximations and computational models recently have been suggested [11–13].

Yttrium aluminium garnet ($2Y_3Al_5O_{12}$, YAG) is now widely used in optical materials because of a variety of unique optical properties. YAG doped with a transition metal or lanthanide ions is an important solid-state laser material [14–18].

We applied our model for estimation of the parameters of the YAG synthesis, such as the diffusion coefficients and reaction rates, using a rather limited information from real laboratory experiments. Namely, the known data only includes the synthesis half-times at different temperatures and synthesis types, and approximate sizes of reactant particles, and energy consumption data, needed to maintain temperature for YAG synthesis. We use the Fick, Arrhenius, and active mass laws. Though the validity of applying the Arrhenius law to heterogeneous reactions has been questioned, the parameters obtained from it often have practical values even if their theoretical interpretation is difficult. In this paper, we mainly consider, the three-dimensional (in space variables) model. The paper is organized as follows. In Sect. 2, we give a brief description of laboratory experiments of YAG synthesis. In Sect. 3, we present a mathematical model for estimation of diffusion-reaction synthesis rates. In Sect. 4, we formulate the main goal of the paper, the parameters to be estimated. In Sect. 5, we present the calculation method and steps, and in Sect. 6, the results obtained in one- and two-dimensional models. In Sect. 7, using the obtained results, we calculate the optimal temperature that minimizes the energy consumption in YAG synthesis. We conclude in Sect. 8. Finally, in Appendix, we give some intermediate numerical results of our calculations.

2 Experimental

The YAG powders could be synthesized by many different methods, such as solid-state reaction, spray-pyrolysis, coprecipitation, sol–gel, and others. The conditions

for the formation of monophasic YAG largely depend on the used synthesis method. For example, by changing the solid-state synthesis method to the sol–gel chemistry approach, the YAG formation temperature decreases from 1,600 °C down to 1,000 °C [19,20].

2.1 Sol–gel method

In the sol–gel synthesis, yttrium oxide was dissolved in 150 mL of 0.2 mol L^{-1} CH$_3$ COOH by stirring the mixture for 10 h at 55–60 °C in a breaker covered with a watch-glass. To this solution, aluminium nitrate dissolved in 50 mL of distilled waster was added, and the resulting mixture was stirred for 2 h at the same temperature. In the next step, 1.2 ethanediol (25 mmol) as complexing agent was added to the above solutions. The acidic medium (pH 5) prevents the flocculation of metal hydroxides in the mixtures and nu adjustment of pH was necessary. After concentrating the solutions by slow evaporation at 60–70 °C under stirring, the Y–Al acetate–nitrate–glycolate solution turned into a white transparent gel. The oven-dried 60–70 °C gel became light brown due to the initial decomposition of nitrates. The gel powders were ground in an agate mortar and preheated for 2 h at 800 °C in air. Since the gels are very combustible, slow heating (2 °C min^{-1}), especially between 150 and 400 °C, was found to be essential. After an intermediate grinding, the powders were additionally sintered at various temperatures from 1,000 to 1,600 °C in air. The optimum annealing time was 5 h at 1,000 °C, 4 h at 1,200 °C, and 3 h at 1,600 °C.

2.2 Solid-state method

In the solid-state reaction method, the stoichiometric mixture of metal oxides (5Al$_2$O$_3$ and 2Y$_2$O$_3$) was carefully ground in an agate mortar and annealed at various temperatures from 1,000 to 1,600 °C in air. The monophasis YAG was obtained only at higher temperature, after sintering oxide precursor for 5 h at 1,600 °C.

3 Mathematical model

We denote by C_3 the concentration of the complex 2Y$_3$Al$_5$O$_{12}$ resulting from the synthesis of two complexes 5Al$_2$O$_3$ and 3Y$_2$O$_3$ with concentrations C_1 and C_2, respectively, in the reaction

$$3Y_2O_3 + 5Al_2O_3 \rightarrow 2Y_3Al_5O_{12}. \tag{1}$$
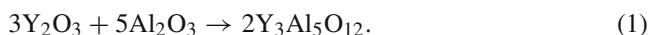
The reaction rate w can be expressed by the rate law as follows:

$$w = kC_1C_2, \tag{2}$$

where k is the reaction rate.

   The dynamics of concentrations of the reactants by diffusion is described by the second Fick's law:

$$w_i = \frac{\partial C_i}{\partial t} = \sum_{j=1}^{3} D_i \frac{\partial^2 C_i}{\partial x_j^2}, \tag{3}$$

where D_i is the diffusion coefficient, n is the dimension of the model, and w_i is the rate of synthesis of the ith reactant. We denote

$$c_1 = 5C_1, \quad c_2 = 3C_2, \quad c_3 = 2C_3; \tag{4}$$

that is, $c_i = c_i(x, t)$ is the concentration of the ith reactant (Y_2O_3, Al_2O_3, $Y_3Al_5O_{12}$ for $i = 1, 2, 3$, respectively) of the synthesis at a point $x \in V$ at time t.

Using the second Fick law and the active mass law for the reaction (1) we get the following partial differential equation system on the synthesis space V:

$$\frac{\partial c_1}{\partial t} = \sum_{j=1}^{3} D_1 \frac{\partial^2 c_1}{\partial x_j^2} - \frac{1}{5} k c_1 c_2, \tag{5}$$

$$\frac{\partial c_2}{\partial t} = \sum_{j=1}^{3} D_2 \frac{\partial^2 c_2}{\partial x_j^2} - \frac{1}{3} k c_1 c_2, \tag{6}$$

$$\frac{\partial c_3}{\partial t} = \sum_{j=1}^{3} D_3 \frac{\partial^2 c_3}{\partial x_j^2} + \frac{2}{15} k c_1 c_2, \tag{7}$$

with initial conditions $c_i(x, 0) = c_i^0(x)$, $x = (x_1, x_2, x_3) \in \overline{V} = V \cup \partial V$, $i = 1, 2, 3$, and some boundary conditions (to be stated below) on the boundary ∂V of V. Since the sizes of molecules Y_2O_3, Al_2O_3, $Y_3Al_5O_{12}$ are nearly the same, we assume that all the diffusion coefficients coincide, that is, $D_1 = D_2 = D_3 = D$. As at high temperatures, the features of solid-state materials change, we think that it is acceptable to apply the methods used for liquids.

We analyze the relations between D and k by using the following data known from the true laboratory experiments at Vilnius University: the synthesis half-times at different temperatures and synthesis methods, and typical dimensions of the reactant particles. By the half-time we mean the time, denoted $t_{1/2}$, in which the total concentration of initial reactants falls to one half; so, it satisfies the equation

$$\int_V (c_1(x, t_{1/2}) + c_2(x, t_{1/2})) dx = \frac{1}{2} \int_V (c_1(x, 0) + c_2(x, 0)) dx. \tag{8}$$

To be concrete, the half-times $t_{1/2}$ approximately equal 5, 4, and 3 h at the temperatures $T = 1,000$, 1,200, and 1,600 °C in the sol–gel synthesis method and 5 h at 1,600 °C in the solid-state synthesis method. At the preparatory stage of the synthesis (using both solid-state and sol–gel reaction methods), the reactants are milled and mixed thoroughly in some cubic volume. The particles in the synthesis space are distributed randomly since their exact initial positions are unknown. As a result,
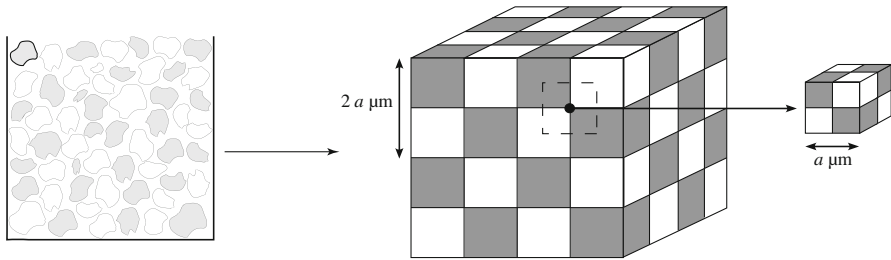
Fig. 1 Synthesis space in the three-dimensional model: $V = (0, a) \times (0, a) \times (0, a)$; $a = 1\,(\mu m)$ for the sol–gel method and $a = \sqrt[3]{10}\,(\mu m)$ for the solid-state method

modeling would require a huge memory size for storage. Therefore, we assume that the are periodically stored in the synthesis volume as shown in Fig. 1. Then, because of periodicity, it suffices to consider the reaction in the cubic synthesis space $V = (0, a) \times (0, a) \times (0, a)$ with zero boundary conditions, $\partial c_i / \partial \mathbf{n}(x) = 0$ for $x \in \partial V$, where $\mathbf{n}$ is the normal vector to the boundary, as shown in Fig. 1. The typical volume of particles is $1\,\mu m^3$ in the sol–gel synthesis method and $10\,\mu m^3$ in the solid-state method. So, summarizing, we arrived at the equation system (5)–(7) in the synthesis space $V = (0, a) \times (0, a) \times (0, a)$ ($n = 3$) with the initial conditions proportional to the initial densities of the particles in the space V and zero boundary conditions, $\frac{\partial c_i}{\partial \mathbf{n}} = 0$ on ∂V.

When solving numerically the partial differential equation system (5)–(7), we use the finite difference technique [21].

4 The main goal

Our estimations are based on the Arrhenius laws describing the temperature dependence of the diffusion and reaction rate coefficients by the following relations:

$$D = D_0 \exp\left\{-\frac{E_D}{RT}\right\}, \quad k = k_0 \exp\left\{-\frac{E_A}{RT}\right\}. \tag{9}$$

Here, E_D is the diffusion activation energy, E_A is the reaction activation energy, D_0 and k_0 are constants, and $R = 8.314472$. Our main goal is to estimate the unknown parameters E_D, E_A, D_0, k_0 by finding the coefficients D and k for temperatures $T = 1,000, 1,200,$ and $1,600\,°C$. In a sense, we solve the inverse problem for system (5)–(7): given the synthesis half-times $t_{1/2}$, we look for the parameters D and k of the system such that the half-time condition (8) is satisfied for all temperatures. Using Eq. (9), for any temperature T, we can find the corresponding parameters D and k, and then, by computer modeling, the corresponding synthesis half-time. This allows us to calculate the energy needed for synthesis at any given temperature and, in particular, to find the optimal temperature.
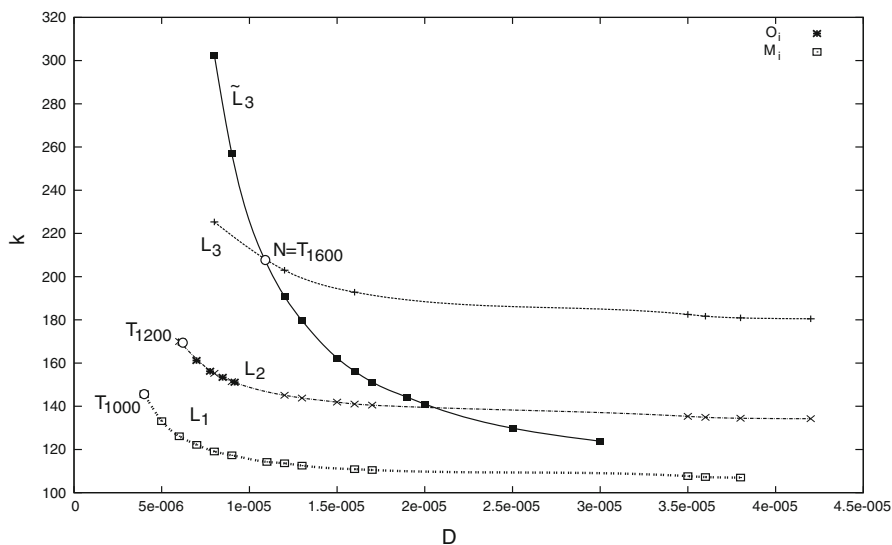
Fig. 2 Calculations in the three-dimensional model. The synthesis space $V = (0, a) \times (0, a) \times (0, a)$; $a = 1$ (μm) for the sol–gel method and $a = \sqrt[3]{10}$ (μm) for the solid-state method

5 Calculation method

We calculate the diffusion and reaction rate coefficients as follows:

First, for each of the temperatures $T_1 = 1,000\,°\text{C}$, $T_2 = 1,200\,°\text{C}$, and $T_3 = 1,600\,°\text{C}$, we draw the graphs L_1, L_2, and L_3 of points (D, k) of the diffusion and reaction rate parameters for which the half-times are equal to those of the laboratory experiments by using the sol–gel synthesis method (i.e., $t_{1/2} = 5$, 4, and 3, respectively). To this end, we use our computer program which, given any fixed D, half-time $t_{1/2}$, and particle size a, numerically solves the system (5)–(7) until the half-time condition (8) is satisfied and, using the middle-point method, finds the value k such that half-time coincides with the given one. A sufficiently large discrete set of the (D, k) values is joined by a smooth curve. Finally, in the same way, we additionally draw the graph $\widetilde{L}_3$ of the (D, k) for the solid-state method ($T_3 = 1,600\,°\text{C}$, $t_{1/2} = 5$). The difference with the previous cases is in the particle-size parameter a, which now takes the value $\sqrt[3]{10}$ (three-dimensional model), instead of $a = 1$. So, in Fig. 2, we see all four graphs: L_1, L_2, and L_3 for the sol–gel method at temperatures T_1, T_2, and T_3; and $\widetilde{L}_3$ for the solid-state method and temperature T_3.

At the same temperature, the values of (D, k) for both synthesis methods coincide. So, the intersection of the graphs $\widetilde{L}_3$ and L_3 gives us the first pair of the true values of (D, k) at the temperature $T_3 = 1,600\,°\text{C}$. We mark by N the intersection point.

To calculate the four unknown parameters (E_D, E_A, D_0, k_0), we need another pair of the values of (D, k). Recall that the graph L_1 is obtained as the spline of m calculated points $M_i = (D_{1000}^i, k_{1000}^i)$, $i = 1, \ldots, m$, obtained by computer modeling, where the main condition was that the half-time is 5 h.

Now, for each pair $N = (D_{1600}, k_{1600})$, $M_i = (D^i_{1000}, k^i_{1000})$, using the Arrhenius law for $T = 1,873$ K and $T = 1,273$ K, we write and solve the following equation system with respect to unknown (E_D, E_A, D_0, k_0):

$$D_{1600} = D_0 \exp\left\{-\frac{E_D}{R \cdot 1873}\right\}, \quad k_{1600} = k_0 \exp\left\{-\frac{E_A}{R \cdot 1873}\right\},$$

$$D^i_{1000} = D^i_0 \exp\left\{-\frac{E^i_D}{R \cdot 1273}\right\}, \quad k^i_{1000} = k^i_0 \exp\left\{-\frac{E^i_A}{R \cdot 1273}\right\}.$$

We denote the corresponding solutions by $(E^i_D, E^i_A, D^i_0, k^i_0)$. Substituting these values of $E^i_D, E^i_A, D^i_0, k^i_0$ into the Arrhenius law (9) with $T = 1200\,°C = 1473$ K, we get a set of points $O_i = (D^i_{1200}, k^i_{1200})$, $i = 1, \ldots, m$.

Now, comparing the points O_i with the graph L_2, we choose the nearest one L_O. Fixing the latter, again from the Arrhenius law, the corresponding unknown E_D, E_A, D_0, k_0 can be found uniquely.

6 Calculation results

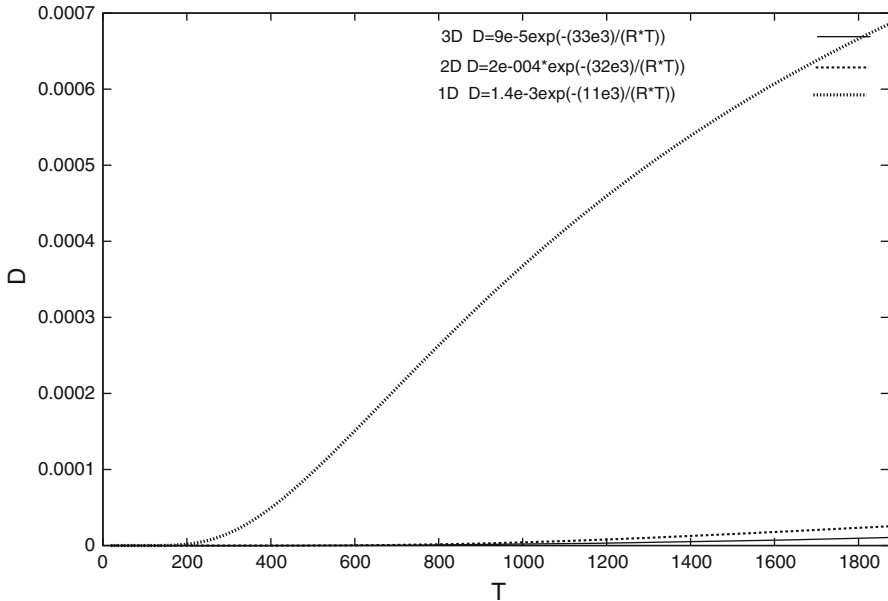For the three-dimensional model, we obtained the following calculation results:

1) $N = (D_{1600}, k_{1600}) = (11\mathrm{e}{-}6, 209)$.
2) $L_O = (6\mathrm{e}{-}6, \ 170)$;
3) The diffusion and reaction rates as functions of synthesis temperature T:

$$D = 9\mathrm{e}{-}5 \exp(-3.3\mathrm{e}4/(RT)), \tag{10}$$
$$k = 450 \exp(-1.2\mathrm{e}4/(RT)). \tag{11}$$

Table 1 Diffusion and reaction rates

T	1,000 °C	1,200 °C	1,600 °C
One-dimensional model			
D	5.0e−4	5.8e−4	7.0e−4
k	113	143	199
Two-dimensional model			
D	10.5e−6	15e−6	28e−6
k	119	146	192
Three-dimensional model			
D	4e−6	6e−6	11e−6
k	146	170	209

3D D=9e-5exp(-(33e3)/(R*T))
2D D=2e-004*exp(-(32e3)/(R*T))
1D D=1.4e-3exp(-(11e3)/(R*T))

Fig. 3 Comparison of dependence of diffusion coefficients on the temperature in one-, two-, and three-dimensional models

The obtained Arrhenius law equations (10)–(11) give us the diffusion and reaction rates at temperatures $T = 1,000$, $1,200$, and $1,600\,°C$, presented in Table 1, where the results in the one- and two- dimensional models [1] are also included for comparison.

The corresponding points (D, k) on the graphs L_1–L_3 and $\widetilde{L}_3$ (Fig. 2) are marked as T_{1000}, T_{1200}, T_{1600}, respectively.

In Figs. 3 and 4, we compare the graphs of the diffusion and reaction rate coefficients as functions of temperature (the Arrhenius law) in all three models.

We see that reaction rate coefficients are rather similar in all models, although the diffusion coefficients are not. The latter difference can be explained by noticing that, in the one-dimensional model, the diffusion actually begins through a single point, while in the two- and three- dimensional models, the "diffusion surface" is essentially larger.

7 Optimization of the energy consumption

Our approach allows us to find the optimal synthesis temperature in the sense of minimal energy consumption. We are given the powers (Table 2, column 3) needed to achieve various temperatures (column 2) in the YAG synthesis. The energy outly was calculated for the high-temperature chamber furnace Nabertherm LHT. From Eqs. (10) and (11) we can get the diffusion and reaction rates (columns 4 and 5) needed for specific temperature and then calculate the corresponding halftimes (column 6) by computer modeling. To calculate the total energy consumption E_T (column 7) under
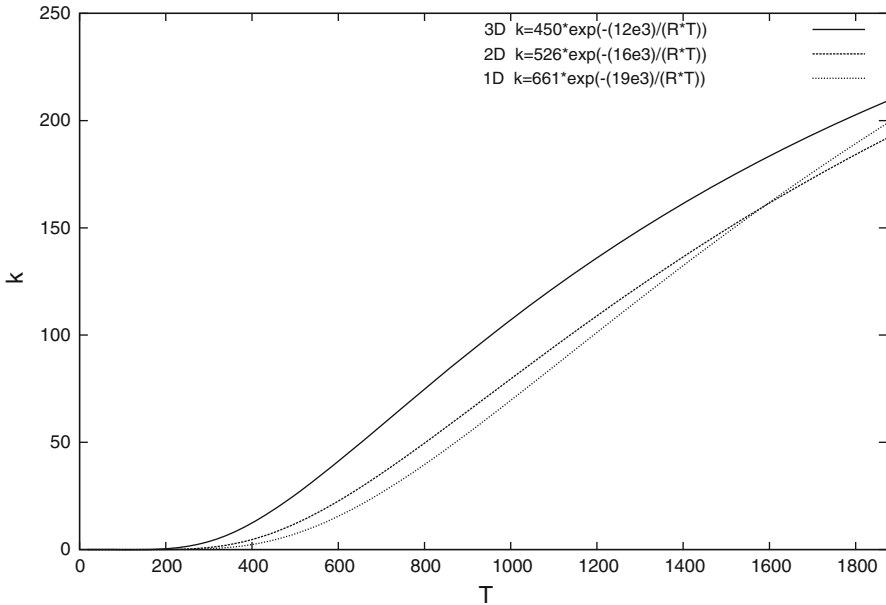
Fig. 4 Comparison of dependence of reaction rate coefficients on the temperature in one-, two-, and three-dimensional models

given synthesis temperature T, we take into account the energy consumed for pre-heating from room temperature, for which the five times higher furnace power is used for half an hour. For simplicity, we assume that the total synthesis time is twice the half-time, although in real experiments, the reaction time is somewhat longer.[1] To be precise, we use the formula

$$E_T = P_T(2.5 + 2t_{1/2}),$$

where P_T is the power used at the synthesis temperature T. Having plotted a graph of energy versus temperature (Fig. 5), we see that the minimal energy consumption in the YAG synthesis is achieved at the temperature $T \approx 1,170\,°C$.

8 Conclusions

Using a mathematical model based on second Fick's, active mass, and Arrhenius laws, we have analyzed a method for calculation of diffusion and reaction-rate coefficients of heterogeneous reactions at high temperatures in the three-dimensional model. First, we have used the half-times of two experiments by different methods at the same fixed temperature. Second, having two additional half-times obtained by the same method at different temperatures:

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[1] Theoretically, the total reaction time is infinite.
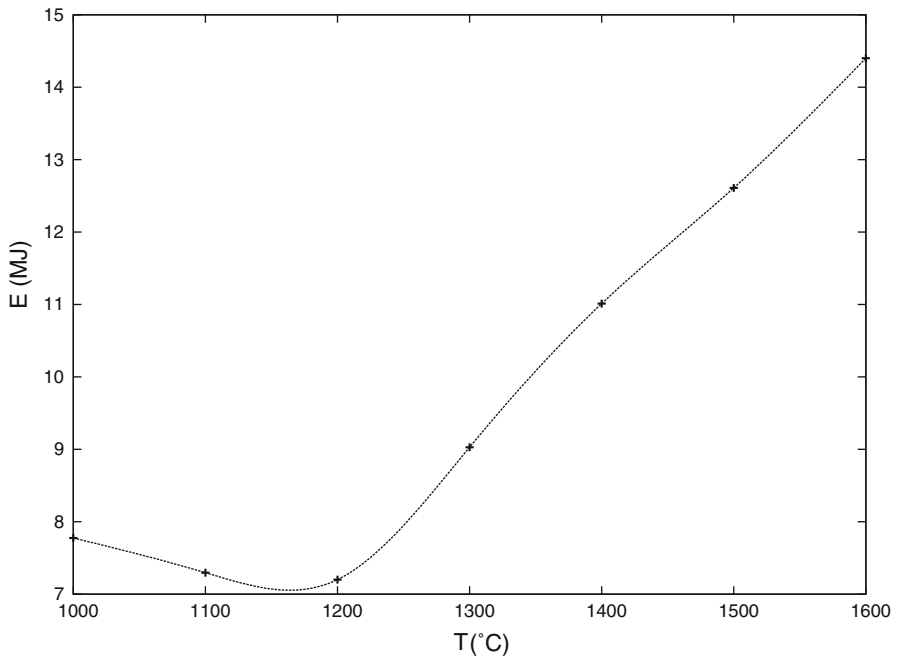
Fig. 5 Energy consumption versus temperature

1. We obtained explicit formulas for the coefficients expressing the dependence of diffusion coefficient and reaction rate on the temperature, provided by Eqs. (10)–(11).
2. At the same time, we have calculated activation energies, important data that can be used to analyze other syntheses.
3. We have compared our results with those of one- and two-dimensional models [1]. For reaction rates, we see similar results in all dimensions. However, for diffusion rates, we the results are similar only for two- and three-dimensional models. Since calculations in the three-dimensional case are significantly more time-consuming than in the two-dimensional case, the two-dimensional model seems to be a good choice for much simpler and less time-consuming calculations.
4. Using Eqs. (10)–(11), we have found the parameters D and k, and using computer modeling, the corresponding half-times for several temperatures. Having them, we calculated the energies consumed at these temperatures and found the optimal temperature.

Appendix: Results of computer modeling

For completeness, we present the intermediate results of calculations obtained when solving the problem. In Table 3, we present the parameters of activation energies of diffusion and reaction E_D^i, E_A^i and constants D_0^i and k_0^i ($i = 1, \ldots, m$) obtained by

Table 2 The energy consumption in YAG synthesis

No.	T (°C)	Power, P_T (kW)	D	k	$t_{1/2}$ (h)	Total energy, E_T (MJ)
1	1,000	648	4e−6	146	5	7.8
2	1,100	667	5e−6	157	4.47	7.3
3	1,200	720	6e−6	170	4	7.2
4	1,300	975	7e−6	181	3.63	9.0
5	1,400	1,260	8e−6	191	3.37	11
6	1,500	1,512	10e−6	200	3.17	13
7	1,600	1,800	11e−6	209	3	14.4

Table 3 Results of three-dimensional modeling

i	M_i		E_D^i	E_A^i	D_0^i	k_0^i	O_i	
	D	k					D	k
1	**4e−6**	**146**	**33e3**	**12e3**	**9e−5**	**450**	**6e−6**	**170**
2	5e−6	133	26e3	15e3	5.9e−5	544	7e−6	161
3	6e−6	126	20e3	17e3	4e−5	611	7.8e−6	156
4	7e−6	122	15e3	18e3	2.9e−5	653	8.5e−6	153
5	8e−6	119	11e3	19e3	2.2e−5	690	9.2e−6	151

our program calculations. Boldface lines show the results chosen under the condition that the point O_i should be the nearest one to the graph L_2.

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