Simulation of Decomposition Kinetics of Supercooled Austenite in Powder Steel

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Abstract. To approve heat treatment of steel modes, quantitative data on austenite decomposition are required. Gaining these data experimentally appears to be extremely complicated. In present work, few approaches to simulate the phase transformation process are proposed considering structure characteristics of powder steels. Results of comparative analysis of these approaches are also given. Predicting the transformation kinetics by simulation is verified for PK40N2M (0.38% C, 2.10% Ni, 0.40% Mo) steel with 3% porosity and PK80 (0.80% C) steel with different porosity using published experimental data.

1. Introduction
Basic patterns of phase transformations in powder steels are similar to patterns observed in forged and cast steels with the appropriate chemical composition [1, 2]. However, it is worth considering that pores are a structural constituent of powder steels, so the porosity strongly affects the decomposition kinetics of austenite. Experimental results allow making a qualitative assessment of this affection [1, 2]. Nevertheless, it is necessary to have accurate quantitative data on phase transformation kinetics to determine scientifically appropriate heat treatment modes. The experimental determination of austenite decomposition diagrams for different steel grades with various porosity is an extremely difficult and very sophisticated process. Math modeling of phase transformations and determination of these diagrams by calculation appear to be reasonable alternatives.

In the literature, attempts have long been known to describe phase transformation kinetics mathematically (e.g., [3 – 6]). Most of the models describe transformation under isothermal conditions based on solidification equation by A.N. Kolmogorov or Avrami equation. However, as it was mentioned in various publications and verified by our research [6], using those equations for modelling transformation during continuous cooling allows one only to gain qualitative correspondence to experimental data. This limitation is particularly due to an unsteadiness period (incubation period) occurring at the abrupt conversion of the system from stable to meta-stable condition. During that unsteadiness period, the probability of new-phase grains formation is determined not by temperature alone [3]. During continuous cooling, system constantly belongs to an unsteadiness period, which was not considered at Kolmogorov or Avrami equations. Thereby, we used another approach to describing phase transformation kinetics based on simulation this process.

2. Discrete simulation of phase transformations
Decomposition of austenite simulation based on solidification scheme by I.L. Mirkin is described in
[6]. This two-dimensional model suggested time discreteness of the process as well as the area, originally occupied by old phase (austenite) discreteness. It was supposed that this area is contingently divided on elementary fragments. The time for which the transformation took place was also divided into elementary intervals. After the end of the unsteadiness period inside the unit of occupied by austenite area, λ elementary fragments were chosen randomly, and every one of them was declared as a new-phase grain. For a time Δt, grains were growing, and lineal speed of their everyway growth was considered as identical and equal l. Time interval Δt was calculated by the following formula:

\[ Δt = \begin{cases} \frac{l_0}{l}, & \text{where } \frac{l_0}{l} < Δt_0, \\ \Delta t_0, & \text{where } \frac{l_0}{l} ≥ Δt_0, \end{cases} \]

where \( l_0 \) is length of elementary fragment, \( Δt_0 \) is elementary time interval. During its growth, each grain attach to itself nearby fragments until a collision to other grains or reaching the border of the area does not occur. In case of collision of growing grains, their growth in the corresponding area stops. Simultaneously, in the area, not occupied by the new phase, grains by the number, proportionate to the area, are appearing. Percentage of not decomposed by the current time austenite was determined as a quotient of area, occupied by the new phase, to all available area.

In this model, kinetics of transformation was determined by the following parameters: unsteadiness period \( τ \), number of grains, appearing in the unit of time inside the unit of area, \( λ \), and linear speed of their growth \( l \). According to the described scheme, the software, which allows one for each given \( τ \), \( λ \) and \( l \) to perform computer experiment, modelling the process of new phase formation and calculating the quotient of decomposed austenite for any time, was developed.

Based on experimentally determined isothermal diagrams [1, 7], by the least square method, numerical values of kinetic parameters of transformation, describing experimental data in the best way, were determined. The values obtained were used for modelling austenite decomposition during continuous cooling.

For each cooling mode a time moment \( t_{727} \), so that \( T(t_{727}) = 727°C \), was determined. From the moment \( t = t_{727} \), an unsteadiness period (during which the transformation did not occur) for this cooling mode was started. It was supposed that from the moment \( t = t_{727} \), during elementary time fragment \( Δt_0 \), sample retention at the constant temperature of 727°C takes place. Then instantaneous cooling to the temperature, calculated according to accepted dependence \( T(t) \), occurs. Then, again, retention during \( Δt_0 \) occurs, etc. In this case, by \( k \) step sum

\[ \frac{Δt_0}{τ(727)} + \frac{Δt_0}{τ(T(t_{727} + 1))} + \ldots + \frac{Δt_0}{τ(T(t_{727} + k - 1))} \]

was calculated, where \( τ(T) \) is the unsteadiness period during isothermal retention at the temperature \( T \). If the determined sum value happens to be not less than \( τ(T(t_{727} + k)) \), then time moment \( t_0 = t_{727} + k \cdot Δt_0 \) was considered as the transformation start time.

After the end of the unsteadiness period, the cooling process continued to be considered as a stepwise process: first, isothermal retention during \( Δt(T) \) occurs; and then instantaneous cooling takes place, etc. Time interval \( Δt(T) \) was calculated using a formula similar to (1) with parameter \( l \), corresponding to given temperature \( T \). On the each step process was considered as isothermal, so for its kinetics describing, simulation, observed above, was used. Considering that new-phase grains can be fully formed only after the end of the unsteadiness period, so the longer this period is, the more noticeably it affects the formation speed of the grains, the number of new-phase grains \( λp(T) \), appearing in the unit of time at the unit of area at the temperature \( T \), was calculated by the following
formula

\[ \lambda_p(T) = \frac{\lambda(T)}{\tau(T)}, \]  

(2)

where \(\lambda(T)\) is the value of the same parameter during isothermal retention at the temperature \(T\), \(\tau(T)\) is the unsteadiness period at temperature \(T\), considering that \(\tau(T) > 1\); otherwise \(\lambda_p(T) = \lambda(T)\). By using the software, which implements described simulation, thermokinetic diagrams for powder steels with different porosity were determined.

As it was shown by the analysis, proposed simulation has various shortcomings. First of all, enlarged volume of processed information (e.g., dividing the original area into smaller elementary fragments or consideration of a three-dimensional model) leads to the abrupt increasing of computer resources, required for the calculation. Next, assumption of discreteness both time and area creates certain difficulties during this scheme implementation.

### 3. Sustained phase transformation simulation (homogeneous origin)

To overcome the shortcomings of discrete simulation, scheme using "from event to event" principle was developed. Under this approach phase transformation should be simulated the following way. At the random moments of time in random dots of three-dimensional, occupied by old phase (austenite) area objects – centers of new phase origin – appears. Each object can occupy area of arbitrary shape.

For ease of the implementation, the ball of given radius \(r_0\) was used. After the new object appears, it begins to grow, herewith the balls' radius increases linearly in course of time. The proposed scheme allows one to consider unsteadiness of origin at the first step: it is supposed, that the grain, which didn't achieve critical size \(r_c\), with certain probability could disappear.

For mathematical description of described processes, the terminology of the queuing theory can be used. Let us consider the system with finite number of channels – possible centers of new phase origin. This can be areas with chemical composition fluctuations, crystal sell defects, etc. At this system, the stream of grains appearance requests arrives. If in the system at the given moment of time there are vacant channels, then the next request will be accepted. In this case, the number of occupied channels will increment by one. Considering unsteadiness of grain origin at the first step, it should be taken into account that before the new-phase grain has a size smaller than critical; the channel serving this request can become vacant with certain probability. Channel may appear to be occupied due to the new request arrival as well as growth of previously formed grains, consuming corresponding area.

Each request is characterized by arrival moment \(\tau_j\) and center coordinates of newly formed object \(\{x_j, y_j, z_j\}\), i.e. can be described by vector of the form \(v_j = v(\tau_j, x_j, y_j, z_j)\). In general, operating with random streams of multidimensional vectors is very difficult, particularly, from the point of view of implementation modelling of this streams. Therefore conventional in simulation of complicated systems practice [8] was used, and number of assumptions was accepted. Particularly, it was accepted that stream \(\{\tau_j\}\) of arrival moment of requests and stream of vectors \(\{x_j, y_j, z_j\}\) can be separately described as independent random objects by corresponding distribution laws. We considered sequence \(\{\tau_j\}\) as a stream of homogeneous events. Based on the assumption of physical patterns of phase transformation this stream can be considered as a stream, which possesses stationary, ordinary and lack of aftereffect properties, so it appears to be elementary (stationary Poisson) stream. Then, according to provisions of the probability theory [8], time between the arrival of two different requests has an exponential distribution with parameter \(\lambda\), where \(\lambda\) is an intensity of the stream. If this intensity was set, following sequence can be obtained: \(t_1, t_2, \ldots, t_k, \ldots\), where \(t_i\) is the time, when the first request arrived, \(t_k, k = 2, 3, \ldots\) is the time between arrival of \((k-1)\) and \(k\) requests. To generate this sequence based on the sequence of quasi-evenly distributed pseudo-random numbers, a known
method, described in [8], can be used. If \( \xi_k, k = 1, 2, 3, \ldots \) are random numbers, evenly distributed on (0, 1), then in order to generate random numbers \( t_k \), exponentially distributed with parameter \( \lambda \), it is reasonable to use the following formula:

\[
t_k = -\frac{1}{\lambda} \ln \xi_k, \quad k = 1, 2, \ldots
\]

(3)

and moments \( \tau_1, \tau_2, \ldots, \tau_k, \ldots \) of requests arrival are expressed by the relations

\[
\tau_1 = t_1, \quad \tau_2 = t_1 + t_2, \quad \ldots \quad \tau_k = t_1 + t_2 + \ldots + t_k, \quad \ldots
\]

(4)

Coordinates of centers of newly generated objects were regarded as independent random values, evenly distributed on the interval, corresponding to the size of considering area. At the moment \( \tau_j \), vector \( \{x_j, y_j, z_j\} \) was generated, and, if the system had a vacant channel, then a new object with a center at \( \{x_j, y_j, z_j\} \) was generated. Otherwise request must be rejected.

The system state as well as the request stream was determined by other two event streams: stream of not reached the critical radius objects decomposition (disappearing) and stream of two (or more) growing objects collision. It was considered that the stream of requests for objects decomposition \( \{\tau^{(d)}_j\} \) also appears to be elementary, so the time between two consistent decompositions has exponential distribution with parameter \( \mu \). After arrival of decomposition request, this request can be accepted only if in the system there are some objects, which are not reached the critical size; otherwise this request must be rejected.

If at the moment of time \( t \), objects \( i \) and \( j \) occupy disjoint areas and have radiuses \( r_i \) and \( r_j \), then the time of their collision can be determined by the following formula:

\[
t_{ij} = \frac{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} - r_i - r_j}{2l},
\]

(5)

where \( r_i = r_0 + l \cdot (t - \tau_i), \quad r_j = r_0 + l \cdot (t - \tau_j), \quad \tau_i \) and \( \tau_j \) are times of generating of objects \( i \) and \( j \), \( l \) is linear speed of their growth.

Hereby, the chain of events was constructed inside the system. Each of events consists either in arrival of request for object generating (or decomposition), or in object collision. If at the moment \( t \) inside the system was generated \( k \) number of objects, then the time up to the next event can be determined by the formula below:

\[
t_e = \min\{t_{k+1}, t_{(d)}^{i,j}, \min_{i,j} t_{ij}\}
\]

(6)

At the moment of the next event occurrence, occupied by new phase volume can be calculated by Monte Carlo method.

Described simulation allows one to significantly reduce required computer resources at the expense of:

- absence of necessity to store in memory information about huge amount of simulated area fragments, as it was in discrete model;

- using the modelling principle "from event to event", which allows to move from discreteness by time to discreteness by events. It reduces the number of system state re-calculating.

Applicability of this simulation to describing austenite decomposition kinetics in powder steels was approved on transformation of PK40N2M steel. Kinetic parameters of the process (such as speed of generating new-phase centers \( \lambda \), linear speed of growth \( l \), intensity of decomposition stream \( \mu \), original size of new-phase grain \( r_0 \) and critical radius \( r_{cr} \)) were selected in order for decomposition curves, determined by the computer simulation, to provide the best description of experimental data [7]. For that purpose for each value of temperature \( T \) of isothermal retention following function was considered
where \((t_i, y_i)\) are points of kinetic curve, determined by an experiment; \(y(\lambda, l, \mu, r_0, r_e, t_i)\) – proportion of austenite, decomposed to the moment \(t_i\) by calculated data, \(n_T\) is the number of experimental points for temperature \(T\). To determine optimal values of kinetic parameters by least square method, the problem was set:

\[
V_{m_T}(\lambda, l, \mu, r_0, r_e) \rightarrow \min .
\]

It is important to notice that the problem (8) has particular characteristics. Firstly, minimized function \(V_{m_T}(\lambda, l, \mu, r_0, r_e)\) was not set analytically. Therefore classical methods of extremum determination, such as Newton method and its modifications, which use the function itself as well as its derivatives of first and second order, are not applicable for this problem. Considering this, for solving problem (8) Hook-Jeeves method was chosen, which is one of the direct search methods, so it uses only values of function itself [9]. According to this method, search of \(m\) variables function minimum consists of sequence of exploring search steps around a basic point towards the changing of one of the variable, then, if succeed, a search by pattern.

Secondly, considering a stochastic nature of observed process it should be taken into account, that the value of the function \(V_{m_T}(\lambda, l, \mu, r_0, r_e)\) with given \(\lambda, l, \mu, r_0, r_e\) and \(T\) appears to be random variable, which value depends on how new-phase grains will distribute inside the considered area. This fact makes application of optimization methods (including Hook-Jeeves method) more difficult, because of the change of the function value, which is expected to be seeing the change of one of the parameters value on each step of optimization, might not exceed range of function values due to the randomness of new-phase grains distribution. To receive correct results of optimization for the determined by static modelling function, using of statistical criteria in verifying inequalities of the form \(V_{m_T}(\lambda^1, l^1, \mu^1, r_0^1, r_e^1) < V_{m_T}(\lambda^2, l^2, \mu^2, r_0^2, r_e^2)\) [8].

In case of problem (8) we used following method. For the same values of kinetic parameters, corresponding to given retention temperature, series of computer experiments (not less than 100), simulated phase transformation, were performed; as a result of it, series of values \(V_{m_T}(\lambda, l, \mu, r_0, r_e), i = 1, 2, \ldots, N\), where \(N\) is the number of experiments in series, was determined. After that, by a random data of obtained sample, mean value \(\overline{V_{m_T}(\lambda, l, \mu, r_0, r_e)}\) and a standard deviation were evaluated, then the hypothesis of significance of \(\overline{V_{m_T}}\) values (obtained on current and previous steps of optimization) difference was verified. To verify this hypothesis, \(t\)-criteria [10], which is regarded to be insensitive to deviations of considered random value from normal distribution (especially in case of huge samples), was used [10].

Based on this method, calculation results showed a possibility of a good approximation of kinetic curves of isothermal transformation. Fig. 1a shows isothermal diagram of PK40N2M steel (porosity 3%), obtained experimentally by magnetometer [7] and results of computer simulation. Besides, form of dependency of kinetic parameter values, obtained by optimization, on the temperature of isothermal retention is well consistent with known theses of heat treatment theories. Therefore these results were used to simulate phase transformations during continuous cooling.

To determine simulation of phase transformations during continuous cooling description of dependency of temperature on time for each cooling mode and dependency of kinetic parameters on temperature (on time for certain mode of cooling) are required. As a basis, experimentally obtained curves of cooling for PK40N2M steel [7] were taken: for each cooling mode series of values \(T_i = T(t_i), i = 1, 2, \ldots, n_k\) was given. These values were approximated by polynomials. For each cooling mode moment of time \(t_{727}\) was determined so that \(T(t_{727}) = 727^\circ\text{C}\). If \(t \in [0, t_{727}]\), then...
temperature of cooling sample remains above critical, so the considered sample resides in region of austenite stability. Therefore, no phase transformation could occur. Starting of the moment of time \( t = t_{277} \), austenite decomposition, simulated by the algorithm above, can occur. Analogically, for each cooling mode was determined moment \( t = t_{M_a} \), where \( M_a \) – is the temperature of martensitic transformation commencement. When considering sample reaching temperature \( M_a \), diffusion speed becomes insufficient for the considered type of phase transformation to occur; therefore inside the framework of this model it was considered that at moment \( t = t_{M_a} \) austenite decomposition by non-martensitic mechanism ends. Thereby, time limits of simulating phase transformation for each cooling mode was determined by segment \( [t_{277}, t_{M_a}] \). Dependency of kinetic parameters on temperature was determined by linear interpolation of values, obtained by solving problem (8).

![Figure 1. Kinetics of austenite decomposition in PK40N2M steel (porosity 3%) according to experiment [7] (1) and simulation (2): a – isothermal diagram; b – thermokinetic diagram.](image)

In case of continuous cooling, intensity of stream of requests for appearance of new-phase grains as well as stream decomposition requests are not constant. Considering that, sequence \( \tau_1, \tau_2, \ldots, \tau_k, \ldots \) of moments of request arrivals may still be constructed by formulas (4), whereas determination algorithm for time intervals between request arrivals \( t_j \) must be modified. For example, in order to determine moment of arrival of the next request following formula should be used:

\[
\int_{t_j}^{t_{j+1}} \lambda(z)dz = -\ln \xi_k, \tag{9}
\]

where \( \xi_k \) are random numbers, evenly distributed at (0, 1), and dependency \( \lambda(t) \) for each cooling mode was constructed by calculation results for isothermal curves.

To determine an occupied by the new phase volume during the continuous cooling, as well as during the isothermal retention, Monte-Carlo method was used. Herewith it was considered, that in case of continuous cooling growing speed of newly appeared objects is not constant and depends on time. Determination of the current radius of grain \( r_j \) was performed according to

\[
r_j(t) = r_0 + \int_{t_j}^{t} l(z)dz, \tag{10}
\]

where dependency \( l(t) \) was preliminary determined for each cooling mode. Results of the simulation and experimentally determined thermokinetic diagram [7], are shown on fig. 1 b.
It should be noticed, that simulation described above was constructed considering homogeneous character of generation (i.e. probability of new-phase centers appearing is equal in every part of non-transformed area), which is, as applied to transformations in powder steels, might be taken as oversimplified. Besides, the presence of powder particles (and, consequently, growth of new-phase grains inside the one particle) and pores existence were not taken into account.

4. Sustained phase transformation simulation (heterogeneous origin)

To overcome limitations mentioned above, certain additional modifications [11] were introduced into simulation:

- Modelled area is divided by fragments (particles). Borders of the particles are set by the equations of planes, each of which has its own number.
- Some amount of particles (depending on the porosity value), are determined as pores.
- At a random moments of time inside random occupied by an old phase areas objects – centers of new phase – are appearing. New-phase grains can possibly appear at
  - the faces of the particles,
  - the borders of the pores,
  and besides, probability of grain appearance at the borders of the pores is significantly higher than at the faces of the particles.
- After new grain appearance, its growth occurs (inside the particle, in which it appeared), herewith grain radius increases linearly with the lapse of time.

Adequacy of determined simulation was evaluated using experimentally obtained isothermal and thermokinetic diagrams for steel containing 0,80% of carbon: forged steel U8 and powder steel PK80 with different porosity [1]. The example of simulation results (thermokinetic diagram for PK80 steel with porosity 15–16%) is shown in fig. 2.

![Figure 2](image)

Figure 2. Thermokinetic diagram for PK80 steel with 15–16% porosity according to experiment [1] (1) and simulation (2).

It is worth mentioning that determined simulation allows predicting decomposition kinetics of austenite for powder steels with different porosities. Particularly, the authors determine optimal values of kinetic parameters for PK80 steel, using experimental data for porosities: 6 – 8% and 26 – 28%. These values without any changes were used to simulate isothermal transformation of the same steel with porosity 15-16%. The results of this simulation are shown in fig. 3.
5. Conclusion

Some approaches to simulate phase transformation during heat treatment of powder steels were proposed. The software implementing this simulations was constructed, which allows one to perform computer experiments, simulating austenite decomposition during isothermal conditions as well as continuous cooling. Analysis of obtained results allows making following conclusions:

- "from event to event" modelling principle, comparing to «\(\Delta t\)» principle, allows one to obtain, on the one hand, more effective simulating algorithms, and, on the other hand, more accurate approximation of experimental data;
- simulation, considering heterogeneous character of new-phase grains generation, allows one to obtain more accurate description of decomposition kinetics of austenite in powder steels than simulation, considering homogeneous character of generation;
- simulation, considering pores as structural components, allows one to predict decomposition kinetics of austenite for different porosities.

References

[1] Ermakov S S, Vyaznikov N F 1990 Powder steels and products. (Leningrad: Mashinostroenie) p 319
[2] Antsiferov V N, Bulanov V Ya, Bogodukhov S I and Grevnov L M 1997 Thermochemical treatment of powder steels. (Yekaterinburg: UrO RAN) p 481
[3] Christian J W 1965 The Theory of Transformations in Metals and Alloys. (Pergamon Press) p 975
[4] Kisino T, Nagaki S and Inoue T 1979 Materials 28(312) 861-867
[5] Mirzayev D A, Okishev K Yu, Schastlivtsev V M, Mirzoev A A, Yakovleva I L and Karzunov S E 1998 Physics of Metals and Metallography 86(6) 590-600
[6] Gurevich Yu G, Ivashko A G and Tsyganova M S 2004 Izvestiya. Ferrous Metallurgy 9 45-48
[7] Gurevich Yu G, Ivashko A G 1998 Kinetics of decomposition of supercooled austenite of powder steels. (Kurgan: Kurgan. gos. univ.) p. 153
[8] Buslenko N P 1978 Modeling of complex systems. (Moscow: Nauka) p 400
[9] Bunday B D 1984 Basic Optimization Methods. (London: Edward Arnold) p 128
[10] Himmelblau D M 1970 Process Analysis by Statistical Methods. (New York: John Wiley & Sons, Inc.) p 463
[11] Ivashko A G, Tsyganova M S and Nabatov R I 2016 Steel in Translation 46(3) 196-200