Prediction of austenite decomposition kinetics in powder steel depending on porosity

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Abstract. For the rationale behind the powder steel heat treatment modes, quantitative data on austenite decomposition kinetics are required. Gaining these data experimentally for different values of porosity is a quite difficult and laborious process. In this article an approach, based on appliance of simulation to evaluation of porosity effect on austenite decomposition kinetics and constructing of isothermal and kinetic diagrams for powder steel by calculation, is proposed. Adaptability of the shown models to predict the transformation kinetics was verified on carbon steel (0.8% C) with different porosity and steel PK45N2 (0.45% C, 2% Ni) with different porosity.

1. Introduction

In order to simulate decomposition kinetics of supercooled austenite and to predict steel structure after heat treatment, experimentally obtained isothermal and thermokinetic diagrams are widely applied. On the one hand, gaining these data experimentally is an extremely laborious process, but on the other hand, using these diagrams in cases when the heat treatment mode significantly differs from the experimental one, is not correct. Concerning that, a lot of mathematical models, predicting the phase transformation kinetics during the steel cooling, were developed [1 – 7]. Most of them describe austenite decomposition under isothermal conditions and are constructed on the basis of the Kolmogorov crystallization equation or the Avrami equation. However, as it was noticed in a number of works and confirmed by our studies [6, 7], applying these equations for simulating transformation during continuous cooling allows one to get only qualitative compliance with experimental data. Particularly, this is due to the presence of the unsteady period (incubatory period) of transformation, during which probability of new phase grains generation under isothermal conditions is determined not only by the temperature [1]. During continuous cooling system constantly stay in unsteady period, and this circumstance is difficult to be taken into account using the Kolmogorov or the Avrami equations. That is why in a number of works (e. g., [6, 7]) simulations of phase transformations of steel were proposed. Particularly, in [7] different approaches to construct simulation of austenite decomposition process (based on discrete and continuous model) were considered. Simulations constructing method allow one to determine the start time and transformation speed, considering unsteadiness.

In case of powder steels, some additional factors, significantly affecting the processes of phase
transformations, which are taking place during cooling or heating, – such as porosity, chemical heterogeneity, causes structural heterogeneity, etc. [8, 9], occur. Studying the effect of these factors on transformation kinetics is of scientific and practical interest in terms of justification of heat treatment modes for powder steels with different porosities.

2. Effect of porosity on transformation in ferritic, pearlitic and bainitic areas

In order to get analytical expressions, reflecting the effect of porosity on kinetic parameters of powder steel austenite decomposition in ferritic, pearlitic and bainitic areas, isothermal and thermokinetic diagrams of transformation in steels of the same chemical composition and different porosities were studied. Quantitative estimates of kinetic parameters of transformation for each value of porosity were made by processing the results of computer experiments, simulating the austenite decomposition process.

Simulation was made based on discrete approach shown in [7] using software developed by us. Transformation under isothermal conditions simulation was performed under the following assumptions. Process kinetics was determined by \( \tau \) – unsteady period, \( \lambda \) – generation intensity of the new phase (number of grains, appearing in the unit of time in the unit of space of the old phase), and \( l \) – linear speed of growth. Nuclear speed of the new phase was assumed as independent of time; linear speed of growth - independent of time and direction of growth (isotropic growth). To determine the values of these kinetic parameters, experimentally gained isothermal diagrams [8, 10] were used: for the trial parameter values series of computer experiments, during which proportion of the transformed space was calculated, was performed. Optimal values were selected to describe in the best way (in terms of the method of least squares) available experimental data. Since classical minimization methods, based on the applying of the gradient of the objective function, could not be used in this case (unknown analytical expression of the objective function), direct search methods were used to determine the required values [11].

It should be noted that, based on the described approach, optimal values of kinetic parameters could be determined only up to a scale factors:

\[
\lambda = \frac{1}{\mu} \cdot \lambda_1, \quad l = \xi \cdot l_1,
\]

where \( \mu \) is a scale factor with unit of measurement \( m^3 \); \( \xi \) is a scale factor with unit of measurement \( m \); values \( \lambda_1 \) and \( l \) are measured in \( s^{-1} \). Generally, after the end of the unsteady period, transformation speed is determined by the value of expression \( \lambda_1 \cdot l_1^3 \), which characterizes space increment of the new phase in the unit of time.

When determining kinetic parameters of powder steels with different porosities, the following considerations were also applied. It is known that the speed of new phase generation is very sensitive to steel structure changes (such as changes of porosity, chemical heterogeneity, structure defects, etc), and linear speed of growth, on the contrary, is a structurally-insensitive factor [8, 9]. So, it was considered that transformation speed increasing, which is observed during porosity increasing, occurring due to increasing of \( \lambda_1 \) - generation speed of the new phase, and decreasing of \( \tau \) - unsteady period, wherein \( l_1 \) - speed of grain growth, does not change during porosity changes.

As a result of several cycles of the computer experiments, values of kinetic parameters of austenite decomposition under different temperatures for carbon steel of 0.8% C with 0%, 6-8%, 15-16% and 26-28% porosity (experimental data from [8] were used), for steel PK45N2 of 0.45% C and 2% Ni with 0%, 5-7% and 14-16% porosity (experimental data from [8] were used) and for steel PK40N2M of 0.38% C, 2.10% Ni and 0.40% Mo with 3% porosity (experimental data from [10] were used), were determined.

Our studies show that gained values of kinetic parameters of transformation can be applied for:

- predicting of transformation kinetics during continuous cooling (results are shown e. g. in [6, 7]);
- obtaining an analytical dependency of kinetic parameters on steel porosity.
To obtain functional dependency of kinetic parameters of austenite decomposition on porosity value, results of simulation, gained for the steel of the same chemical composition, but different porosity, were analyzed. Since it was previously assumed that there is no significant dependence of the linear speed of grains growth on porosity, it was sufficient to describe the effect of porosity on the speed of new phase centers generation and on the unsteady period.

Dependence of the new phase centers generation speed on porosity is proposed to be described using the following functions:

\[
\lambda_1(\theta) = \lambda_1(0) + a \cdot \left(1 - e^{b \cdot \theta}ight),
\]

where \(\lambda_1(0)\) is the speed of new phase centers generation in the compact steel of the same composition; \(\theta\) is the value of porosity, \%; \(a\), \(b\) and \(n\) are coefficients depending on temperature of isothermal aging of steel.

Experimental data on austenite isothermic decomposition in steels of the same chemical composition with different porosities (e.g., [8]) show that effect of the porosity on process kinetics significantly depends on aging temperature. Thus, at temperatures of the least stability of austenite, transformation speed in steel with 14-16% porosity increases several times comparing to compact steel, and in upper perlitic area at temperature 680-700°C, it increases hundreds of times. That is why parameters \(a\), \(b\) and \(n\) in equation (2) were determined separately for different values of temperature. In table 1 the obtained values of these parameters for carbon steel of 0.8% C are shown.

**Table 1.** Dependence of parameter \(a\), \(b\) and \(n\) on isothermal aging temperature for steel of 0.8% C.

| Temperature, °C | \(a\), s\(^{-1}\) | \(b\) | \(n\) |
|----------------|-----------------|------|------|
| 350            | 8597.0          | -9.0 \(\cdot\) 10\(^{-6}\) | 4.30 |
| 400            | 8599.9          | -9.52 \(\cdot\) 10\(^{-6}\) | 4.30 |
| 450            | 8600.0          | -1.32 \(\cdot\) 10\(^{-5}\) | 4.20 |
| 500            | 8649.7          | -2.40 \(\cdot\) 10\(^{-5}\) | 3.99 |
| 550            | 8646.5          | -2.99 \(\cdot\) 10\(^{-5}\) | 3.93 |
| 620            | 8620.0          | -2.0 \(\cdot\) 10\(^{-6}\) | 4.90 |
| 650            | 8500.0          | -8.51 \(\cdot\) 10\(^{-7}\) | 5.0  |
| 680            | 5500.0          | -2.66 \(\cdot\) 10\(^{-8}\) | 6.0  |

Figure 1 illustrates the nature of the obtained dependence (markers show values of parameter \(\lambda_1\), which were determined previously by simulation).

Dependence of unsteady period at a given temperature on porosity is proposed to be described by the following function:

\[
\tau(\theta) = \tau(0) \cdot e^{b_1 \cdot \theta^{n_1}},
\]

where \(\tau(0)\) is an unsteady period for compact steel with the same composition and under the same temperature; \(\theta\) is porosity value, \%; \(b_1\) and \(n_1\) are coefficients depending on isothermal aging temperature. These coefficients, as well as parameters of the equation (2), were determined separately for different temperature values. Table 2 contains gained values of these parameters for carbon steel of 0.8% C.

Figure 2 illustrates the nature of the obtained dependence (markers show values of parameter \(\tau\), which were determined previously by simulation).
Figure 1. Dependence of parameter $\lambda_1$ on porosity for steel of 0.8% C.

Table 2. Dependence of parameters $b_1$ and $n_1$ on isothermal aging temperature for steel of 0.8% C.

| Temperature, °C | Parameters | Parameters |
|----------------|------------|------------|
|                | $b_1$      | $n_1$      |
| 350            | -0.4678    | 0.39       |
| 400            | -0.1257    | 0.72       |
| 450            | -0.0289    | 1.08       |
| 500            | -0.0277    | 1.06       |
| 550            | -0.0194    | 1.06       |
| 620            | -0.0489    | 1.03       |
| 650            | -0.060     | 1.0        |
| 680            | -0.0456    | 0.92       |

Figure 2. Dependence of parameter $\tau$ on porosity for steel of 0.8% C.
Similar calculations for coefficients of equations (2) and (3) values were performed for steel PK45N2 with different values of porosity. Obtained results allow predicting transformation kinetics for those values of porosity, for which there are no experimental data. Results of that prediction for carbon steel with 10% porosity are show in Figure 3. For comparison, some experimental data for close values of porosity are also given.

Figure 3. Isothermal diagrams for steel of 0.8% C with different porosity.

3. Effect of porosity on transformation in martensitic area
The simulation shown below is almost inapplicable for studying martensitic transformation kinetics, because the speed of martensite growth by far exceeds the speed of new phase centers generation, which, as it is known, is determined by free energy gain during the new phase generation.

It is noted in papers [8, 12] that in porosity steels, as well as in compact materials, the position of point $M_n$ (point of the beginning of martensitic transformation) does not depend on cooling speed. In [12], it is shown experimentally that for number of powder steels, temperature of the beginning of the martensitic transformation grows linearly with the porosity growth. Authors of [12], analyzing thermodynamic characteristics of $\gamma \rightarrow \alpha$ transformation in porous powder steels, explain this dependence by decreasing of elastic energy with increasing of porosity. To determine the free energy gain during the new phase (martensite) centers generation, coherently related to matrix under hydrostatic pressure, in [2] the following equation was obtained:

$$\Delta \Phi = \left( \Delta \Phi_0 + 3P \alpha + \frac{E \alpha^2}{1 - \nu_n} \right) \cdot \frac{4}{3} \pi r^3 + \sigma \cdot 4 \pi r^2,$$

$$\Delta \Phi_0 = \Phi_0^1 - \Phi_0^2,$$

where $\Phi_0^1$ and $\Phi_0^2$ – thermodynamic potentials without intension of new and old phases, resp. (J); $P$ – hydrostatic pressure on the system (Pa); $\alpha = \frac{1}{3} \frac{\Delta V}{V}$ – a dilatation effect of phase transformation;
$\Delta V$ – a volume effect of transformation; $E$ – a modulus of elasticity (Pa); $v_n$ – Poisson coefficient; $\sigma$ – surface tension force, (J/m$^2$); $\rho_{cr}$ – critical radius of the new phase grain, (m).

In equation (4) the third summand inside brackets determines increasing of elastic energy during dilatation effect. The greater it becomes, the smaller becomes absolute value of $\Delta \Phi$, ergo, the smaller becomes speed of new phase centers generation. It is known [13, 14] that the modulus of elasticity is related to porosity by the following relation:

$$E = E_c \cdot \theta^m,$$

where $E_c$ is the modulus of elasticity of compact material (Pa); $\theta$ is relative density; $m = 1.5, \ ... , 2$ is the coefficient. Poisson coefficient is determined by the relation:

$$v_n = \nu^{m} \cdot v_{nc},$$

where $v_{nc}$ is Poisson coefficient for compact solid; $m = 0.25, \ ... , 0.5$.

Thereby, modulus of elasticity and Poisson coefficient are decreasing with porosity increasing, which leads to increasing of free energy gain, ergo, increasing of probability of martensite generation centers appearance. Furthermore, porosity increasing displaces the temperature of phase equilibrium of martensite and austenite, which is determined as the solution of the following equation:

$$\Delta \Phi_0(T) + \frac{E \cdot \alpha^2}{1-v_n} = 0.$$

For predicting formation kinetics of martensite grains generation centers, dependence of free energy gain relative permutation on porosity was evaluated, according to (5) and (6). Results of this evaluation show that for steel with porosity 5%, 10% and 15% relative increasing of centers generation speed is, respectively 7.9%, 14.9% and 21%. It is consistent with the experimental data shown in Figure 3.

4. Conclusion

- Simulation system of austenite decomposition in ferrite, perlite and bainite areas [6, 7] can be applied for evaluation of porosity effect on transformation kinetics in powder steels. In this paper, equations describing dependence of kinetic parameters on porosity were proposed.
- Appliance of obtained relations in common with simulation of austenite decomposition allows predicting transformation kinetics for those porosity values, for which there are no experimental data.
- Porosity effect on austenite decomposition speed in martensitic area can be determined by evaluation of free energy gain during new phase generation. It was shown that dependence of martensite grain generation speed on porosity can be approximately considered as linear.

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