ARCH. MECH. TECH. MATER. VOL. 38 (2018) 35-39

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# Austenite transformation simulation for a controlled rolling processing technology development

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**ARTICLE INFO**

Received 18 July 2017
Received in revised form 24 May 2018
Accepted 06 June 2018

**KEY WORDS**

phase transformation,
controlled rolling,
computer simulation

**ABSTRACT**

Using an originally-developed computer model and appropriate software the impact of deformation on austenite phase transformation in low carbon alloyed steel was carried out. The computer simulation takes into account an impact of the deformation degree and takes into account non- constant cooling rate. That makes it useful for the development of thermal and deformation technological processes development. Based on the simulation results a technology of controlled rolling of low carbon steel alloyed by carbide forming elements (Nb, V, Ti) was developed. The proposed technique allows production of rolled steel sheets with high strength and plastic properties, as well as high impact strength in normal and low temperatures.

## 1. INTRODUCTION

Deformation and heat treatment technologies, in particular controlled rolling, are widely used for obtaining optimal structural characteristics and high mechanical properties of steel rolling sheets. These techniques regulate the degrees and temperature intervals of deformation, as well as the cooling rate. A more pronounced effect could be achieved using a two-stage deformation regime, which involves high-temperature deformation and a cleaner lower temperature deformation that precedes the phase transformations or occurs during them [1, 2, 3]. Experimental-only methods usually used for controlled rolling technologies development could be effective but they are time, material and energy consuming. Nowadays, computer simulation is becoming more widespread in different scientific and technical areas. Good examples of simulation implementation in material science and metallurgy, especially for deformation and heat treatment processes, are given in works by [4, 5, 6].

We developed a physical-based semi-empirical mathematical model for phase transformation kinetics simulation and appropriate software [7, 8]. The essence of the model is given in works [9, 10] and references there. This model is based on physical and mathematical description of nucleation and growth of phases which could be the products of austenite transformation (ferrite, cementite (including one in perlite), bainite, martensite and special carbides) and elements redistribution between phases. Thermodynamic calculation of phase equilibrium (CALPHAD-method) is also included in the model. An important point is that the cooling rate could be given as non-constant and non-linear in time for the simulated process conditions (by a time/temperature table). The developed model also takes into account the degree of austenite pre-deformation, which is important for simulation of the phase transformation in controlled rolling technological processes. The data about temperature changes could be experimental or also simulated by heat transfer modelling. The modelling results and the model reliability were experimentally proofed [9, 10].

DOI: 10.2478/amtm-2018-0006

## 2. STUDIED MATERIAL

The investigated material was a low-carbon steel alloyed by Mn and also containing Mo and Si, and micro alloyed by V and Nb and traces of Ti, which formed specific carbides. The steel composition in simulations is given in table 1. The initial austenite average grain size was set to 50 μm.

**Table 1, The steel's chemical composition (in wt. %)**

| Fe | C | Mn | Si | Mo | V | Nb | Ti | N |
|---|---|---|---|---|---|---|---|---|
| base | 0.08 | 1.60 | 0.20 | 0.16 | 0.05 | 0.04 | 0.02 | 0.003 |

This type of steel is used for higher strength rolled sheets with good weldability manufacture. Controlled rolling technology is typically used for obtaining high structure quality and appropriate strength and plastic properties.

## 3. METHODOLOGY AND BASE THEORY

Ferrite transformation kinetics modelling is based on works by [5, 11]. Equations which describe the model of phase transformations kinetics theoretical base were given in our work [9]. The model essence is to describe the rates of nucleation and grows of the phases occur during austenite transformation (ferrite, cementite, bainite, martensite). But these equations do not take into account the influence of deformation. According to works [5, 11] the ferrite nucleation inside austenite grains in not deformed metal was not considered due to its insignificant rate. Only ferrite nucleation on the faces, ribs and vertices of austenite grains was considered. The origination of perlite in eutectic steels occurs at the boundaries of austenite grains. In low- and medium-carbon steels, it begins in carbon-rich interphase regions. The limiting process with the growth of perlite colony is the volume diffusion of carbon in austenite [5]. As a leading phase in a pearlite colony grows process cementite carbide was considered.

The subject of this paper is the influence of the deformation on phase transformation kinetics which was not considered in our previous works. It is known that a preliminary deformation of austenite accelerates the process of its decay and leads to a significant grinding of the finite microstructure [11]. The reason for the acceleration of decay is the activation of ferrite grains nucleation along the boundaries of the austenite grains [12] and the stimulation of additional nucleation on the deformed substructure within the austenitic grains [13].

In the existing models of ferrite transformation the influence of deformation is taken into account, the corresponding change in the number of places of origin, as well as the increase of the vibrational force of the process by increasing the energy of austenite after its deformation.

The number of works that physically substantiate and describe the effect of the previous deformation on the decay of austenite is rather small [5].

Ferrite nucleation by the third (inner grain) mode is described by the similar to other modes of the transformation process equation (1):

$$J_i = C_i \cdot N_i^0(t) \frac{1}{\sqrt{T}} e^{-\frac{Q_N(Y_{AE})}{RT}} \cdot e^{-\frac{(K_i \cdot \sigma_{eff})^3}{k_B \cdot T \cdot \Delta G^2_{\gamma\to\alpha}(T,Y_{AE})}} \quad (1)$$

where: $J_i$ – rate of ferrite nucleation by i-th process mode, $1/s \cdot m^2$; $C_i$ - empirical factor, which takes into account the influence of a crystal lattice defects rate in the certain place on the atoms moving rate, $K^{1/2}/s \cdot m^3$; $N_i^0(t)$ - the amount of potential nucleation places by the moment; T – temperature, K; $Q_N(Y_{AE})$ – the activation energy of the $\gamma \to \alpha$ lattice rebuilding, J/mol; R – universal gas constant, J/mol·K; $K_i$ – empirical coefficients; $\sigma_{eff}$ – the effective surface energy of a ferrite, $J/\cdot m^2$; $k_B$ – Boltzmann constant, J/K; $\Delta G_{\gamma\to\alpha}(T, Y_{AE})$ – change of the volumetric Gibbs energy in $\gamma\to\alpha$ transformation as a function of the chemical composition and temperature, $J/m^3$.

Parameter $K_i$ from the equation (1) for inner grain nucleation was calculated by formula (2):

$$K_i = K_{i0} - q_\varepsilon \cdot \sigma_0 \cdot \varepsilon \quad (2)$$

where $K_{i0}$ – shape factor [10, 11] as it in not deformed metal; $q_\varepsilon$ – empiric parameter, $\sigma_0$ - level of internal stresses after deformation; ε – deformation degree.

The description of the austenite deformation influence on phase transformation kinetics in our model is based on works [4, 5, 11]. The mode of the ferrite nucleation inside grains becomes significant in deformed austenite [11]. In our model, we assumed that the places of origin of the intragrain ferrite are predominantly austenite subgrains boundaries, and the rate of its nucleation depends on the size of the subgrain and the fraction of the large-angle boundaries. The average size of subgrains was estimated by the equation (3) from [11]:

$$d_\varepsilon = k_{\varepsilon 1} \cdot \frac{\nu \cdot \mu(T_\varepsilon) \cdot b}{\sigma_0} \quad (3)$$

where: $k_{\varepsilon 1}$ – an empirical parameter taking into account the stress relaxation at the moment of transformation, ν – Poisson's ratio, μ ($T_\varepsilon$) – shear modulus at the deformation temperature, b – Burgers vector modulus, $\sigma_0$ – internal stresses after deformation.

The fraction of large-angle boundaries was calculated from formulas (4, 5) from [5, 11]:

$$\delta_\varepsilon = 1 - e^{-\left(\frac{\varepsilon}{b(T)}\right)^3} \quad (4)$$

$$b(T) = 0{,}5 \cdot e^{\frac{T_\varepsilon - 850}{400}} \quad (5)$$

where: $T_\varepsilon$ - deformation temperature.

The level of internal stresses after deformation was estimated by an empirical formula (6):

$$\sigma_0 = 22{,}7 \cdot \varepsilon^{0{,}271} \cdot d_\gamma^{-0.07} \cdot e^{\frac{2880}{T_\varepsilon}} \quad (6)$$

where: ε – deformation degree, $d_\gamma$ – austenite grain size, $T_\varepsilon$ – deformation temperature.

Coefficient $C_i$ from equation (1) for the third mode also depends on the deformation according to formula (7):

$$C_3 = C_{30} \cdot \delta_\varepsilon \cdot \sigma_0 \cdot \frac{1}{a^3} \quad (7)$$

where $C_{30}$ – empirical factor; $\delta_\varepsilon$ - average size of subgrains; $\sigma_0$ – internal stresses after deformation; a – lattice parameter.

Briefly the schema of calculation organization and synchronization of modelling of various types transformations is given below. The possibility of the process of the ferrite transformation is considered by the model, provided that the temperature of the system is lower than $A_3$, the equilibrium between austenite and ferrite is not achieved, pearlite transformation does not begin. The conditions for completing of a ferritic transformation modelling may be: achieving a phase relation between the ferrite/austenite close to the equilibrium (only if the system is not further removed from an equilibrium), beginning of a pearlitic transformation, the achievement of a conditional artificial criterion for calculating the temperature or time limit (the latter concerns all other pre-rotations). Perlite and ferrite transformation can not proceed simultaneously. The pearlite transformation begins to be taken into consideration below $A_1$ when the concentration of carbon in austenite is at least as important for the formation of perlite at a given temperature. The criteria for the simulation of pearlite transformation completing may be: complete (or almost complete) completion of the transformation of austenite, the achievement of artificial limits by temperature or time. The distance between plates in perlite is determined during the simulation by formula 8.

$$S_{\theta\alpha} = -\frac{4 \cdot \sigma_{\alpha/\theta}}{\Delta G_{\gamma\to\theta}(T, Y_{AE})}, \quad (8)$$

where $\sigma_{\alpha/\theta}$ - the specific energy of the α/θ - boundary; $\Delta G_{\gamma\to\theta}(T, Y_{AE})$ - change in Gibbs energy during the formation of cementite from austenite.

At values of the calculated inter-plate distance less than 0.4 microns, the structures were assigned to fine pearlite. For large ones, they were considered as an ordinary perlite.

The criterion of the possibility a banetic transformation start is achieving the value of Gibbs energy change of γ→α the transformation was this value below $\Delta G_{sh.} \sim 500$ J/mol However, the formation of ferrite (if the formation of perlite has not begun) is not excluded. Its formation can occur in the early stages of the formation of bainite and actually ends with further decrease in temperature and suppression of diffusion processes. Perlite transformation was also not excluded from the calculation when the bainite transformation process was simulated. But in fact it is also suspended due to low diffusion at low temperatures. The rate of formation of martensite elements was based on instantaneousity. Its amount depends from the current composition and temperature (formula 9):

$$f_M = 1 - e^{-m\cdot(M_S - T)^n} \quad (9)$$

where $M_S$ – the temperature of the onset of the martensitic transformation, depending on the chemical composition of the austenite, K; m, n – parameters depending on the chemical composition.

The calculation of bainite, ferrite or perlite transformations did not formally stopped when considering of martensitic one, but in fact their speed is already very low.

## 4. THE MODEL VERIFICATION

Some experimental testing for the developed model validation were carried out and already described in works by [8, 9]. New verification experiments were made recently. Their results are shown below. The steel composition assumed in the experimental testing is given in table 2.

***Table 2, The steel's chemical composition in the verification experiments (in wt. %)***

| Fe | C | Mn | Si | Mo | Cu | Ni |
|---|---|---|---|---|---|---|
| base | 0.053 | 1.20 | 0.32 | 0.26 | 0.45 | 2.42 |

A distinctive feature of these experiments and simulation is redecoration of the metal and austenite strain accounting. The steel samples were pre-deformed at temperature 1050 – 1070 °C with deformation degree about 30 %. The cooling rates were kept constant and there values were: 5, 10, 17 and 30 °C/s. A number of dilatometric tests were carried out for an experimental study of the decay of supercooled austenite. In these tests cylindrical metal samples cut from steels of the appropriate composition, were subjected to heating and cooling according to a given thermal regime. During the heating and cooling, a change in the diameter of the sample was measured by a fast-acting dilatometer.

A comparison of calculated kinetic curves of austenite transformation with experimental points is shown on figure 1. The plots show that there is resemblance between experimental data and results of computer simulation. Thus although computer simulation is not a complete alternative to experimental research, it allows us to obtain data that are reliable enough for the technician. It is useful for the development of a steel heat and deformation treatment technology.

## 5. RESULTS AND DISCUSSION

Phase transformations at deformation and cooling process were studied using the developed model. The studied controlled rolling regime includes the next stages: high temperature deformation (where austenite recrystallization occurs); faster cooling to temperatures close to equilibrium ferrite transformation; final deformation before the actual transformation process beginning (at the incubation period); faster cooling to the actual pearlite transformation; slower cooling to the pearlite transformation ending; non controlled air cooling. Computer simulation was used to predict the equilibrium and actual transformation beginning and ending temperatures, as well as the determination of optimal cooling rates. Out thermodynamic calculation predicted that the values of critical points (steel composition from table 1) are as follows: $A_3$ = 864 °C, $A_1$ = 726 °C. Especially when subjected to fast cooling, actual temperatures of transformation start are significantly lower.

A calculation experiment was carried out to determine the optimal cooling regime for ferrite-pearlite (with minor bainite amount) structure with small ferrite grains sizes. The numerical parameters of the proposed regime are as follows. High temperature deformation in the interval 1200 – 1130 °C executed with summary deformation degree at least 50 %. At higher than this temperature interval carbide forming elements (V, Nb, Ti) are mostly dissolved in the austenite (thermodynamic calculation). In this interval carbides of Nb and Ti partially precipitate which prevents grain grows. The occurring austenite recrystallization leads to forming not elongated but globular and small austenite grains. Then metal cooled with rate of 5 – 8 °C/s to 830 °C. Then the final deformation executed with degree of 40 – 70 %. The ending

temperature of the final deformation is 760 °C. Then metal cooled to 650 °C with rate 4 – 7 °C/s. After that the cooling rate slowed to 0.1 – 0.3 °C/s before the metal temperature becomes 520 °C. In this period pearlite and fine disperse special carbides are forming. After that the phase transformation are already completed, so in the next period the cooling could be not controlled in the free air.

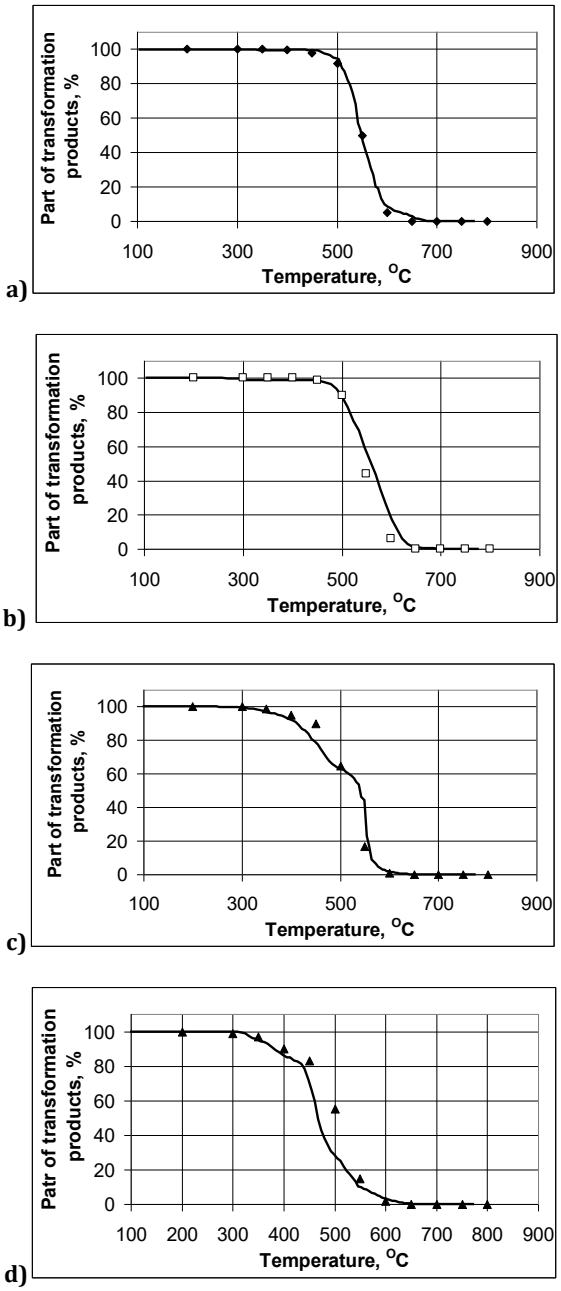


***Fig. 1 Comparison of calculated kinetic curves (given as solid lines) of austenite transformation with experimental data (given as points) at different constant cooling rates: a) 5 °C/s, b) 10 °C/s, c) 17 °C/s, d) 30 °C/s***

The simulated kinetic curve of austenite transformation during the described above cooling regime are shown below on figure 2. There also shown a curve of a similar regime but without deformation. For simulations of transformations in a not deformed sample a model as in our works [9, 10] was used. In the model which consideres deformation the inner grain (in subgrains boundaries) mode of nucleation was included. Actually both models are integrate in the same program product [10] and share some common modules.

The deformation makes ferrite transformation go faster, especially at the ending period. It leads to finer ferrite grains because of more active nucleation (including nucleation inside grains).

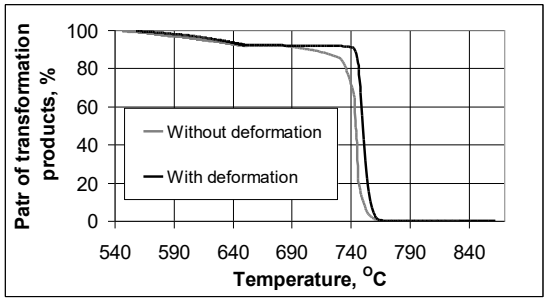


***Fig. 2, Simulated cooling curves of austenite transformation during studied cooling regime***

The actual start temperature of ferrite transformation is about 760 °C. At this temperature the final deformation ends. The temperature of actual pearlite transformation beginning is about 650 °C. When this temperature is exceeded, the cooling rate should be fast enough to prevent carbides forming but slow enough for ferrite transformation to complete. Then slowing of cooling to 0.1 – 0.3 °C/s is enough to complete of pearlite and carbides formation higher then 520 °C to prevent bainite forming which is rather brittle and not equilibrium phase.

The mechanical properties of steel samples obtained by the proposed regime are given in table 3 below.

***Table 3, Mechanical properties of the steel samples after controlled rolling***

| | $\sigma_B$, MPa | $\sigma_T$, MPa | δ, % | Ψ, % | Impact strength KCU, MJ/m$^2$ | | KCV, MJ/m$^2$ |
|---|---|---|---|---|---|---|---|
| | | | | | + 20 °C | - 60 °C | -15 °C |
| Minimum | 782 | 644 | 24 | 62 | 2.37 | 1,33 | 1.45 |
| Maximum | 798 | 675 | 35 | 69 | 2.64 | 1,52 | 1.65 |
| Average | 787.8 | 656.3 | 29.4 | 65.6 | 2.48 | 1.46 | 1.64 |

Thus, the proposed method allows obtaining steel of grade X70 class (approaching the X80), significantly improving both strength and plastic properties and impact strength at normal and lower temperatures.

## 6. CONCLUSIONS

Using computer simulation by originally developed software austenite transformation processes in low-carbon steel was studied. The simulation took into account the impact of austenite deformation on ferrite nucleation kinetics. It was shown that this impact is significant enough and previous deformation leads to more fine ferrite structure also because of fastening of ferrite nucleation process and innergrain nucleation activation. Another factor is austenite

recrystallization at high temperature deformation that generates finer austenite grains.

The developed model was used for simulation of austenite transformation in controlled rolling processing and post deformation cooling. The calculation experiment allowed defining and optimizing values of temperature ranges and cooling rates in the controlled rolling technology. The proposed technique leads to obtaining of fine ferrite structure and high enough strength and plastic properties of low-carbon steel micro alloyed with strong carbide forming elements (Ti, Nb, V).

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