

Computer simulation of microstructure transformation in heat treatment processes

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co-operating with

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Analysis and modelling

ABSTRACT

Purpose: Most often used methods for prediction of austenite decomposition are described and analysed.

Design/methodology/approach: The austenite decomposition prediction is usually based on continuous cooling transformation (CCT) diagrams. The next method is based on semi-empirical approach based on the Scheil's additivity rule. The third method is based on time, $t_{8/5}$, relevant for microstructure transformation measured on Jominy-specimen. Very good results are obtained by artificial neural network (ANN) with learning rule based on the error backpropagation algorithm.

Findings: By the comparison of application ability of investigated methods in mathematical modelling and computer simulation of austenite decomposition during the cooling of low-alloyed steel, it can be concluded that everyone method gives different results, and minimum variation in elemental composition and history of cooling may produce extremely different results in microstructure portion. Very good results were achieved by the method, which applies the Jominy-test results. In this method the additivity rule and specific performance of Jominy-test has been combined.

Research limitations/implications: The investigation was performed on low-alloyed steels.

Practical implications: The results of prediction of microstructure transformations could be used for prediction of mechanical properties after a heat treatment and of generation of stresses and strains during a heat treatment.

Originality/value: The ability and applicability of potential methods of austenite decomposition prediction in general mathematical modelling of heat treatment of steel are carried out. The finding of this paper will be so useful in development new algorithms in mathematical modelling and computer simulation of heat treatment of low-alloyed steels.

Keywords: Artificial intelligence methods; Computer simulation; Microstructure transformation; Cooling; Additivity rule

1. Introduction

Heat treatment is a process in which products made of metals and alloys are upon thermally in order to change their structure

and properties in the desired direction. One of the main problems with which the theory of heat treatment is considered, is how the microstructure of metals and alloys is related with their properties of engineering importance. Heating or cooling of a metal can

change its microstructure, which causes variations in the mechanical and physical properties, and affects the behaviour of the metal in processing and operation.

The properties of steels can be influenced in a wide range by changing the thermodynamical properties by suppression of the equilibrium states during cooling [1].

During a very slow cooling of steel, austenite decomposition is controlled by diffusion of iron, carbon and alloying elements, and therefore time-dependent. Cooling of austenite with increased cooling rates gives no chance to finish diffusion processes, the transformation temperatures are lowered, and austenite transforms diffusionless.

An important consideration in many of the heat treatments is the variation in cooling rate between the surface and center of heat-treated parts. The differential cooling produces stresses that may cause distortion and even cracking.

Prediction of microstructure transformations is prerequisite for successful prediction of mechanical properties after a heat treatment and of generation of stresses and strains during a heat treatment. Phase transformation modelling is one of the main challenges in modelling of heat treatment [2].

In this paper four most often used methods for prediction of austenite decomposition are described and analysed. The main method is based on continuous cooling transformation (CCT) diagrams. The next method is based on semi-empirical approach based on the Scheil's additivity rule. The third method of austenite decomposition prediction is based on time, $t_{8/5}$, relevant for microstructure transformation measured on *Jominy*-specimen. Very good results are obtained by using artificial neural network (ANN) with learning rule based on the error backpropagation algorithm.

2. General approach

The microstructure transformations during cooling have been extensively investigated experimentally and theoretically. The most often used method in prediction of austenite decomposition during the cooling is based on isothermal transformation (IT) or continuous cooling transformation (CCT) diagrams. CCT diagrams are irreplaceable in the clear presentation of microstructure transformation during the steel cooling in order to predict microstructure composition and hardness after the cooling, but results of austenite decomposition depend on concrete history of heat treating process [3].

On the other hand, many mathematical models based on fundamentals of thermodynamics and kinetics have been developed to evaluate kinetics of austenite decomposition as well as to predict the effect of cooling rate and austenite structure on final microstructure and achieved mechanical properties of the products.

The microstructure transformation kinetics started to be intensive investigated in 1930-ties, when Kolmogorov [4] had developed first kinetics model of austenite decomposition based on nucleation and growing rate of a new phase. However, the most often cited in this field are the works of Johnson and Mehl [5] and Avrami [6]. Many investigations have proved that those models could be efficiently used for simulation of isothermal, diffusion-controlled austenite decomposition. For the calculation of the transformed austenite during diffusionless transformation of austenite to martensite, model proposed by Koistinen and Marburger [7] is widely used in literature.

Many scientists [8-15] had continued afore-mentioned investigations in purpose of developing mathematical models that will provide better results of austenite decomposition prediction during isothermal holding, as well as continuous cooling. In investigation of austenite decomposition during continuous cooling, most often the cooling curve is approximated with a series of isothermal holding, where, for calculation of new phase fractions, Scheil's additivity rule is applied.

Prediction of microstructure based on *Jominy*-test results is combination of mathematical modelling and experimental testing. Time of cooling from 800 to 500°C, $t_{8/5}$, is relevant for microstructure transformation in most structural steels. By involving the time $t_{8/5}$ in the mathematical model, the *Jominy*-test results could be included in the model [16-17].

Artificial Neural Networks (ANNs) represent different approach of investigation of microstructure transformation. The use of ANNs has increased over the past 10 years in materials science [18-22] due to achieved good results of prediction. After learning the relationship between input and output data, the ANN becomes able to generate output data for any new input value. This method is very suitable for prediction of materials properties in case when some of the relevant factors are unknown, as well as for solving complex phenomena for which physical models do not exist.

3. Prediction of austenite decomposition

3.1. CCT diagram

Most heat treatments of steels involve the continuous cooling of a specimen to room temperature. During continuous cooling, the transformation is spread over a wide range of temperatures and ferrite, pearlite, bainite and martensite may be observed in specimen.

In Figure 1 the cooling curve of investigated heat treating process is shown. It can be expected that with this heat treating process microstructure composition will consist of ferrite, pearlite, bainite and martensite.

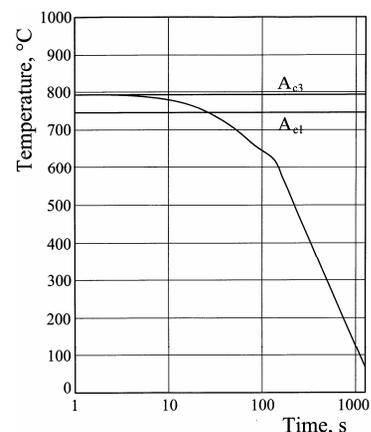


Fig. 1. Cooling curve

Figure 2 shows CCT diagrams of low-alloyed steel 34Cr4 (DIN), as well as cooling curves and related hardness in HRC or HV after the cooling of two different chemical compositions (Table 1).

Table 1.
Chemical composition of the investigated steels

Chemical composition	Mass concentration of the alloying element, %			
	% C	% Si	% Mn	% Cr
I	0.35	0.23	0.65	1.11
II	0.36	0.29	0.69	1.09

According to Figure 2, the cooling rate has decisive influence on the microstructure obtained. At high cooling rates austenite transforms only to martensite, at low cooling rates ferrite and pearlite are obtained, at medium cooling rates microstructures of ferrite, pearlite, bainite and martensite arise. By changing the cooling rate from extremely slow to extremely fast, the hardness can be changed for example from 180 HV to 56 HRC (Figure 2a).

Austenite decomposition is defined by both the cooling time from 800 to 500 °C, $t_{8/5}$, and the shape of the cooling curves in the CCT diagrams. For the same time $t_{8/5}$ the microstructure obtained during

continuous cooling may be quite different if a constant cooling rate or an exponential time-temperature cycle is applied [1]. CCT diagrams are only valid for the time-temperature cycle used in the actual test.

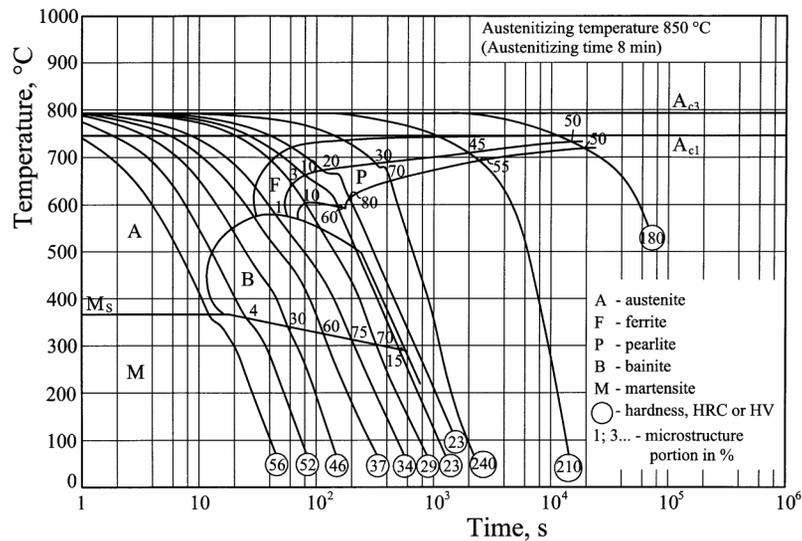
Therefore, disadvantage of CCT diagram method is in discrepancy of cooling curves of real cooling process and cooling curves of CCT diagram. Small discrepancy of cooling curves at the beginning of cooling could cause large deviation between cooled engineering component and specimen used for CCT diagram construction.

CCT diagrams do not take into consideration history of heat treatment and state of materials.

Advantages of application of CCT diagrams are in their simplicity and certainty.

Table 2 gives the microstructure composition of steel 34Cr4 of two different chemical compositions after the cooling from austenitizing to room temperature in accordance with cooling curve shown in Figure 1.

a)



b)

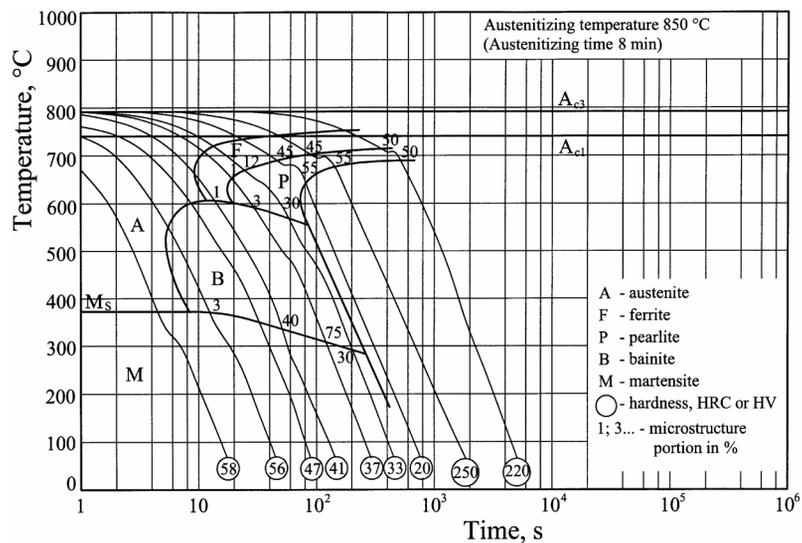


Fig. 2. Continuous cooling transformation (CCT) diagrams of steel 34Cr4: a) chemical composition I, b) chemical composition II [3]

Table 2.
Prediction of microstructure composition by CCT diagrams

Chemical composition	Microstructure composition, %		
	ferrite + pearlite	bainite	martensite
I	13	70	17
II	100	0	0

By application of two different CCT diagrams of steels with very similar chemical composition, extremely different results of microstructure composition has been achieved.

3.2. Additivity rule based on IT diagram

For the isothermal transformation, there is a general agreement on the validity of the Johnson-Mehl-Avrami transformation equation [9] that gives the volume fraction X of austenite transformed as the function of the constant temperature, T and of the time, t :

$$X = 1 - \exp(-k t^n) \quad (1)$$

where k and n are the rate constant and the time exponent, respectively. The transformed fraction X in an isothermal transformation is a function of time. The rate constant depends on the temperature and transformation mechanism. The time exponent is a constant in the temperature range when a unique transformation mechanism operates [15]. Equation (1) is valid for diffusion-controlled austenite decomposition.

The prediction of austenite decomposition during a continuous cooling is still one of the main challenges in modelling of heat treatment. The question arises of relating continuous cooling, i.e. non-isothermal transformations to the isothermal transformations, in order to take advantage of the good knowledge available for the latter. This is often accomplished with the help of the Scheil's additivity rule [1, 9, 10, 15]:

$$\int_0^t \frac{dt}{\tau(X_0, T)} = 1 \quad (2)$$

where $\tau(X_0, T)$ represent the isothermal transformation time for $X = X_0$ at a temperature T , and t is the total transformation time.

According to additivity rule, the non-isothermal transformation kinetics can be described as the sum of a series of the small isothermal transformations.

Figure 3 shows the scheme for microstructure prediction from cooling curve and an isothermal diagram. In figure, the temperature range is divided into a series of small finite steps. Maintaining the time interval, Δt_i to sufficiently short times permits the assumption that the conditions are isothermal over each time step.

It was assumed that each time step produces such a transformation as occurs in the isothermal diagram at the same temperature. Furthermore, it was accepted that the rate of austenite decomposition is constant during the cooling process.

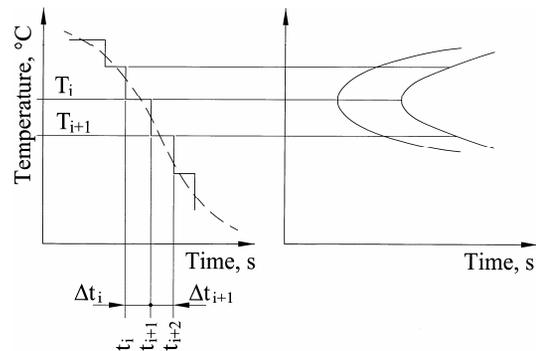


Fig. 3. Microstructure composition prediction from cooling curve and IT diagram

The volume fraction ΔX of austenite transformed in the time interval Δt_i at temperature T_i can be calculated as follows:

$$\Delta X = \frac{\Delta t_i}{\tau(T_i)} \quad (3)$$

where $\tau(T_i)$ is the isothermal transformation time at a temperature T_i .

Additivity rule is complex method, which should take in account the variation of transformation rate in various period of cooling.

Table 3 gives microstructure composition of steel 34Cr4 after the cooling from austenitizing to room temperature in accordance with cooling curve shown in Figure 1.

Table 3.
Prediction of microstructure composition by additivity rule based on IT diagram

Chemical composition	Microstructure composition, %		
	ferrite + pearlite	bainite	martensite
I	30	62	8

3.3. Application of additivity rule with Jominy test result

Microstructure composition after the cooling depends on actual steel hardness. It can be written that the steel hardness is generally equal:

$$HV = ((\% \text{ferrite})HV_{(F)} + (\% \text{pearlite})HV_{(P)} + (\% \text{bainite})HV_{(B)} + (\% \text{martensite})HV_{(M)})/100 \quad (4)$$

In addition, the amount of phases fraction is equal unity:

$$((\% \text{ferrite} + \% \text{pearlite}) + (\% \text{bainite} + \% \text{martensite})/100 = 1 \quad (5)$$

By the equations (4) and (5) is not difficult to predict phases fraction if both, hardness (HV) of cooling microstructure with 90% or 50% of martensite and of 10%, 50% or 90% of (ferrite+pearlite), as well as hardness of microstructure constituents separately are known.

Results of austenite decomposition are depending on the chemical composition of steel, severity of cooling, austenitizing temperature and steel history.

The austenite decomposition results can be estimated based on time relevant for microstructure transformation. The characteristic cooling time relevant for microstructure transformation for most structural steels is the time of cooling from 800 to 500 °C, time $t_{8/5}$ [3]. Involving the time $t_{8/5}$ in the mathematical model of steel cooling, the Jominy-test results can be involved in austenite decomposition model.

Everyone location of *Jominy*-specimen has one characteristic time $t_{8/5}$. The diagram distance from the quenched end of *Jominy*-specimen (*Jominy*-distance) vs. cooling time $t_{8/5}$ is shown in Figure 4 [3].

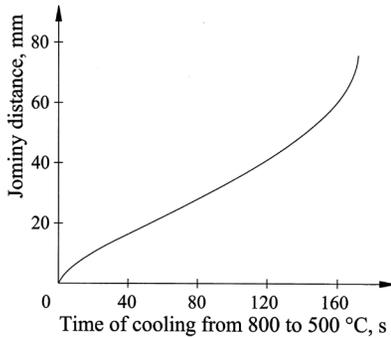


Fig. 4. *Jominy*-distance vs. cooling time from 800 to 500°C

If other heat treatment parameters are constant, the austenite decomposition results in some location of a cooled specimen depend only of the time $t_{8/5}$.

It could be written for *Jominy*-test that phase hardness depends of chemical composition (CC), and cooling rate parameter (CRP), that corresponds to actual distance from the quenched end of *Jominy*-specimen, d . It was adopted that $CRP = t_{8/5}$.

$$HV_d^M = f_M(CC, CRP) = HV_{max}^M - K_M \log \frac{t_{8/5d}^M}{t_{8/5max}^M} \quad (6)$$

$$HV_d^B = f_B(CC, CRP) = HV_{max}^B - K_B \log \frac{t_{8/5d}^B}{t_{8/5max}^B} \quad (7)$$

$$HV_d^{P+F} = f_{P+F}(CC, CRP) = HV_N^{P+F} + K_{P+F} \log \frac{t_{8/5N}^{P+F}}{t_{8/5d}^{P+F}} \quad (8)$$

where HV_d^M is the hardness of martensite at the distance d from the quenched end, HV_{max}^M is the maximal hardness of martensite, HV_d^B is the hardness of bainite at the distance d , HV_{max}^B is the maximal hardness of bainite, HV_d^{P+F} is the hardness of pearlite and ferrite at the distance d , and HV_N^{P+F} is the hardness of pearlite and ferrite in normalized state. Characteristic values of hardnesses HV , coefficients K and times $t_{8/5}$ in equations (6), (7) and (8) have to be evaluated based on chemical composition of investigated steel combined by *Jominy*-test results.

Hardness of quenched microstructures with 100%, 90% or 50% of martensite can be predicted by using the diagram of hardness at different percentages of martensite vs. carbon content after Hodge and Orehoski [1, 23] and by *Jominy*-curve diagram, but the influence of chemical composition of steel has to be taken in account.

Distances from the quenched end of *Jominy*-specimen with martensite fraction of 90% and 50% can be predicted by *Jominy*-curve diagram, by conversion of hardness results to distances.

Distances of 100% of martensite and of 100% of pearlite can be predicted by the *Jominy*-curve.

The regression relations between the cooling time from 800 to 500°C for cooling microstructures of 100%, 50%, 10% and 0% of pearlite and ferrite are established [17].

$$\log \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{90\%(P+F)}} = f_{90}(CC, T_a, t_a) \quad (9)$$

$$\log \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{50\%(P+F)}} = f_{50}(CC, T_a, t_a) \quad (10)$$

$$\log \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{10\%(P+F)}} = f_{10}(CC, T_a, t_a) \quad (11)$$

$$\log \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{0\%(P+F)}} = f_0(CC, T_a, t_a) \quad (12)$$

where T_a is the austenitizing temperature in K, and t_a is the austenitizing time in hours.

Characteristic *Jominy*-distances for characteristic time $t_{8/5}$ can be estimated using the relation between cooling time and distance from the quenched end of *Jominy*-specimen shown in Figure 4.

Jominy-test method applies the additivity rule and assumes matching of cooling curves of real cooling process and cooling curves of CCT diagram. Prediction error of this method could be partially reduced by taking in account the hardness value.

The phase fraction of *Jominy*-specimen of steel 34Cr4 is estimated by computer simulation. *Jominy*-test results are shown on Figure 5. Chemical composition of steel 34Cr4 is 0.36 % C, 0.28 % Si, 0.63 % Mn, and 1.15 % Cr. Austenitizing temperature was equal 850°C.

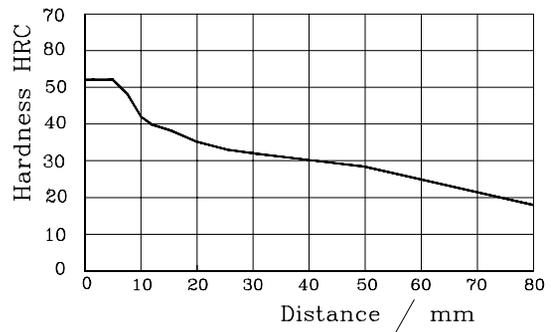


Fig. 5. *Jominy*-curve off steel 34Cr4

Diagram of simulated microstructure composition for *Jominy*-specimen of steel 34Cr4 is shown on Figure 6. Prediction of austenite decomposition results by *Jominy*-test method was done in accordance with cooling curve shown in Figure 1.

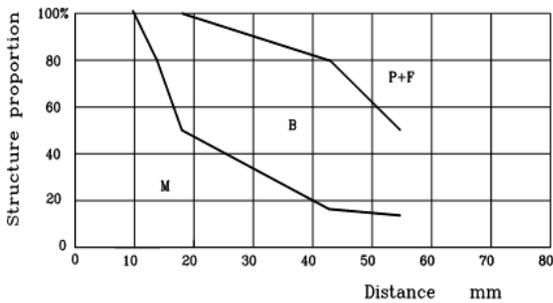


Fig. 6. Microstructure fraction vs. *Jominy*-distances

Table 4 gives microstructure composition of steel 34Cr4 after the cooling from austenitizing to room temperature (Figure 6).

Table 4.
Prediction of microstructure composition by application of additivity rule with *Jominy*-test results

Microstructure composition, %		
ferrite + pearlite	bainite	martensite
37	49	14

Comparison of applied methods in prediction of microstructure composition of cooled steel 34Cr4 is shown in Table 5.

Table 5.
Comparison of microstructure composition results

Prediction method	Microstructure composition, %		
	ferrite + pearlite	bainite	martensite
CCT diagram I	13	70	17
CCT diagram II	100	0	0
A. r. & IT d.	30	62	8
A. r. & <i>Jominy</i> -test	37	49	14

3.4. Artificial neural network

Besides the given methods, the authors suggest the ANN approach in the prediction of microstructure transformation during the steel cooling. The static multi layer feed forward ANN with learning rule based on the error backpropagation algorithm, with momentum and adaptive learning rate, has been applied.

Every ANN has an input layer, one or more hidden layers and one output layer. The number of network inputs and the number of network outputs are constrained by the problem that has to be solved. The number of hidden layers between network input and output layer, as well as the number of neurons in hidden layers, is up to designer.

The basic mathematical principle of learning by experience in ANN corresponds to a nonlinear procedure that maps an input vector to an output vector by using free parameters that are called weights and biases. The learning process is performed by comparing the

desired values and actual values obtained by ANN in order to minimize the sum-squared error of the ANN, i.e. the goal function E :

$$E = \frac{1}{2} \sum_{n=1}^N (d_n - O_n)^2 \quad (13)$$

where N is the size of the learning dataset, d_n is the desired response, and O_n is the actual response of the ANN.

The change of the network weights and biases is given by expressions:

$$\mathcal{A}(n+1) = \mathcal{A}(n) + \Delta \mathcal{A}(n) \quad (14)$$

$$\Delta \mathcal{A} = -\eta \frac{\partial E(\mathcal{A})}{\partial \mathcal{A}} \quad (15)$$

where $\mathcal{A}(n+1)$ and $\mathcal{A}(n)$ are new and old value of parameters, respectively, and η is the learning rate coefficient.

The dataset for learning and testing of ANN is taken from [3]. The input data of ANN are the chemical composition: %C, %Si, %Mn, %Cr, %Mo, %Ni, the austenitizing temperature, T_a , the austenitizing time, t_a , the total hardness of cooled steel, HV_1 and the time of cooling from 800°C to 500°C. The output data of ANN are the fractions of ferrite and pearlite, $F+P$ and of martensite, M . The fraction of bainite, B is subsequently calculated by equation:

$$\% B = 100 \% - (\% (F + P) + \% M) \quad (16)$$

The dataset for learning of ANN is consisted of nine low-alloyed steels. More information is given elsewhere [22]. The dataset for testing of ANN is given in Table 6.

Different network topologies were tested, and the best one with one hidden layer and the 10-5-2 topology with log-sigmoid transfer function with bias was assumed for the calculation. The learning rate of the neural network was set to 0.01, whereas the learning rate increment and decrement were set to 1.05 and 0.7, respectively. The degree of momentum was set to 0.95. The error ratio, which determines the ratio of new error to old error, was set to 1.04. The maximum number of epochs to learn was 30000, and acceptable level of sum-squared error was 0.3.

Results of prediction of microstructure composition after the cooling of steels 16MnCr5*, 15CrNi6**, and 18CrNi8* of testing dataset are given on Figure 7, Figure 8, and Figure 9, respectively.

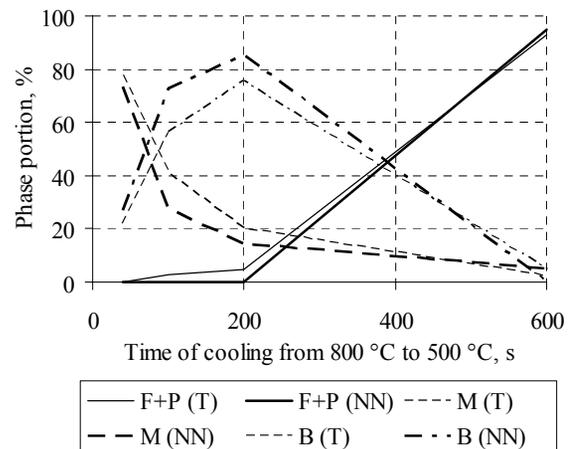


Fig. 7. Microstructure composition of 16MnCr5

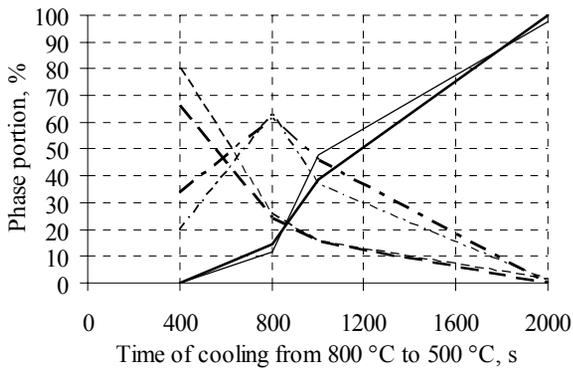


Fig. 8. Microstructure composition of 15CrNi6**

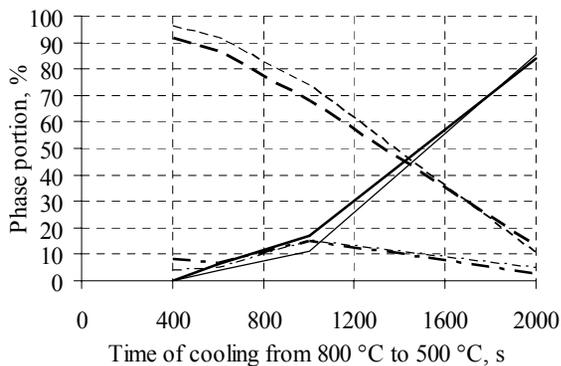


Fig. 9. Microstructure composition of 18CrNi8*

Table 6. Testing dataset

	Ck15*	16MnCr5*	15CrNi6**	18CrNi8*	14NiCr14
C %	0.30	0.33	0.50	0.56	0.13
Si %	0.29	0.22	0.31	0.31	0.26
Mn %	0.39	1.12	0.51	0.50	0.46
Cr %	0.12	0.99	1.50	1.95	0.78
Mo %	0.00	0.02	0.06	0.03	0.04
Ni %	0.00	0.12	1.55	2.02	3.69
T_a °C	830	830	830	830	1050
t_a min.	15	15	15	15	15
HV_t	547	516	600	748	414
	415	400	469	716	277
	293	348	412	649	256
	240	291	304	436	200
$t_{8/5}$ s	1	40	400	400	10
	4	100	800	600	200
	8	200	1000	1000	1000
			2000	40000	

* or ** Composition of carbon in steels is obtained by adding the carbon in standard low-carbon steel.

4. Conclusions

Microstructure transformation causes variations in the mechanical and physical properties, and affects the behaviour of the metal in processing and operation. Microstructure transformation prediction is one of the main challenges in modelling of heat treatment.

In this paper four most often used methods for prediction of austenite decomposition was described and analysed. The main method is based on continuous cooling transformation (CCT) diagrams. The next method is based on semi-empirical approach based on the Scheil's additivity rule. The third method of austenite decomposition prediction is based on time, $t_{8/5}$, relevant for microstructure transformation measured on *Jominy*-specimen. Very good results are obtained by using artificial neural network (ANN) with learning rule based on the error backpropagation algorithm.

Good results of prediction of microstructure transformations were achieved by application of CCT diagrams. These diagrams are irreplaceable in the clear presentation of microstructure transformation during the steel cooling in order to predict microstructure composition and hardness after the cooling, but results of austenite decomposition depend on concrete history of heat treating process. Extremely different results of microstructure composition were achieved by application of two different CCT diagrams of steels with very similar chemical composition.

The modified Johnson-Mehl-Avrami transformation equation was analyzed, which is based on Scheil's additivity rule. In application of additivity rule the non-isothermal transformation kinetics was described as the sum of a series of the small isothermal transformations.

By the comparison of application ability of investigated methods in mathematical modelling and computer simulation of austenite decomposition during the cooling of low-alloyed steel, it can be concluded that everyone method gives different results, and minimum variation in chemical composition and history of cooling may produce extremely different results in microstructure fraction. Very good results were achieved by the method, which applies the *Jominy*-test results. In this method the additivity rule and specific performance of *Jominy*-test has been combined.

The ANN approach in prediction of microstructure transformation during the steel cooling was described very useful. The static multi layer feed forward ANN with learning rule based on the error backpropagation algorithm, with momentum and adaptive learning rate, has been applied.

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