DETERMINATION OF AUSTENITE DECOMPOSITION TEMPERATURES USING THERMODYNAMIC SW FACTSAGE

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Abstract

The article will deal with the determination of austenite decomposition temperatures using the available SW FactSage. The determination of austenite decomposition temperatures is one of the basic information that can provide the technologist and subsequently help to change the properties of steel during steel processing. Austenite is one of the interstitial carbon solutions. Austenite is characterized by a cubic area-centered lattice and its structure is formed by regular grains. Various phases or structural components may form during cooling of austenite. Depending on the cooling of the steel, perlite, bainite and martensite may be formed. During the cooling of the steel, the area-centered lattice changes to a spatially centered iron lattice alfa. The aim of the presented work will be to determine the decomposition temperatures of austenite in 41Cr4 steel.

Keywords: Steel, FactSage, austenite, transformation, temperature

1. INTRODUCTION

For the changing world market of the steel industry, which uses other technological processes of steel production, knowledge of austenite decomposition temperatures is very important for understanding the basic properties of steel. Modern economical production and processing of steel as well as constantly meeting the customer's requirements for the quality of the steel produced require accurate information on the austenite decomposition products for a given steel grade [1].

An important area of application of the knowledge of phase transformation temperatures is the solidification of steel, because the transformations that occur in the steel during its cooling are one of the decisive factors that most affect the final properties of the steel. In particular, austenite transformations at different cooling rates and different degrees of subcooling are of great practical importance for the heat treatment of steel. Individual types of transformations (peritectic, bainitic, martensitic) differ in the course and decomposition products of austenite. After heat treatment, we get steels with different physical properties [1,2].

As the cooling rate increases, the phase transformations take place at lower temperatures than those corresponding to the equilibrium diagram [2]. Upon accelerated cooling, austenite transforms into perlite at a lower temperature and in a range of carbon concentrations, which increases with increasing cooling rate (further increase in cooling rate leads to martensitic conversion) [3]. Another parameter that affects austenite decomposition temperatures is pressure. As the pressure increases, the solubility of carbon in austenite decreases and the temperature of the beginning and end of austenite decomposition decreases [3,4].

The aim of the presented technical article is to determine the austenite decomposition temperature (Ac1 and Ac3) using the FactSage software. Based on the calculation, a regression analysis will be compiled using a regression equation, which will be determined using Microsoft Excel 2016.

2. AUSTENITICAL PHASES

Austenite is an equilibrium structural component existing at higher temperatures in polymorphic steels. As mentioned above, austenite is formed by the transformation of a ferritic-cementitic structure, which is referred to as the austenitization process. Two processes are important in this process, namely austenite homogenization and austenitic grain growth [4].

Various phases or structural components may be formed during cooling of the austenite. The basis of the ongoing transformations is, under equilibrium conditions, the change of the cubic surface-centered iron lattice γ to the spatially centered iron lattice α, the carbon content is also reduced, and cementite is formed. Diffusion of iron atoms is required for allotropic conversion of the iron lattice, and carbon diffusion is required for carbon redistribution and carbide formation. Both processes are affected by the transformation temperature [4,5].

The pearlitic transformation is the transformation of austenite that occurs during its slow cooling (or at a higher temperature of isothermal endurance). Under equilibrium conditions and at eutectoid concentration, perlite is formed from austenite, which is a mixture of ferrite and cementite. The growth of perlite is thus conditioned by the formation of germs of both phases. This conversion is diffuse, and the growth rate of perlite does not depend on time but increases with increasing supercooling. As austenite subcooling increases, the amount of cementite and the thickness of the pearlitic lamellae decreases. The pearlitic transformation is significantly influenced by the additive elements, which in most cases slow down this transformation. The resulting perlite reaches the lowest hardness of the possible austenite transformations [6,7].

The bainitic transformation takes place during medium-rapid cooling (or at medium isothermal holding temperature), at temperatures below about 550 °C and above the martensitic transformation temperature. Bainite is formed, which consists of ferrite (which is formed by the shear mechanism) and cementite (which is formed by the diffusion mechanism). With the transformation temperature and with the chemical composition of austenite, the structure of the emerging bainite also changes; we distinguish between the so-called upper and lower bainite. The structure of lower bainite is, in contrast to perlite, harder and has a finer structure [7,8,9].

The martensitic transformation occurs during rapid cooling of austenite, the maximum rate at which diffusion transformations are still suppressed is referred to as the critical cooling rate. This transformation produces martensite, which is a supersaturated solid solution of carbon in iron α, due to its high carbon content, martensite has a high hardness. It is formed without diffusion transformation by a shear mechanism (i.e., the chemical composition of martensite will be the same as the composition of the starting austenite). The temperature at which the martensitic transformation begins does not depend on the cooling rate of the austenite but it is a function of the state of the austenite (especially its chemical composition) [7,8,9].

3. DETERMINATION OF AUSTENITE DECOMPOSITION TEMPERATURE

The literature data are mostly limited to specific steel types and are insufficient to determine the thermodynamic properties of steel, especially depending on temperature. In the publications, the authors limit themselves to constant values of thermophysical quantities for a specific temperature. Thermodynamic properties can be further determined according to empirical equations [10]. These are mainly regression equations, which were constructed based on empirical research. Here, too, restrictions apply about the studied chemical composition of steel. Another of the mentioned methods can be, for example, the determination of thermophysical properties of steels using the pseudo-binary phase diagram Fe-C mentioned in [11].

FactSage SW was used to determine the Ac3 and Ac1 decomposition temperatures of austenites in 41Cr4 steel grade. The chemical composition of the steel can be seen from **Table 1**. **Figure 1** shows an austenite decomposition graph showing Ac3 and Ac1 temperatures for 41Cr4 steel. The database FSstel was chosen to determine austenite decomposition temperatures for steel 41Cr3. The average temperature Ac3 is 770 °C and Ac1 is 740 °C. The calculated temperatures vary by up to 30 °C depending on the chemical composition. The austenite decomposition takes place in undereutectoid steels (with a carbon content of 0.02 wt.).

The temperatures of Ac3 and Ac1 can be affected by the presence of individual elements in the steel. The Ni, Mn or C elements are austenitic, thus expanding the austenite region and thus lowering the onset and end temperatures of austenite decomposition. On the contrary, elements such as Si or S belong to the ferrite-forming ones, they narrow the region of austenite and thus increase the temperature of the beginning and end of austenite decomposition (P and Cu behave in the same way). Cr is also one of the ferrite-forming elements, but it increases the end temperature of the austenite decomposition and decreases the temperature of the austenite decomposition.

Table 1 Chemical composition of 41Cr4 steel

	C	**Si**	**Mn**	**P**	**S**	**Cr**
	0.38 - 0.45	**≤ 0.40**	**0.6 - 0.9**	**≤ 0.025**	**≤ 0.035**	**0.9 - 1.2**
min.	0.38	0.00	0.60	0.00	0.00	0.90
avg.	0.42	0.20	0.75	0.01	0.02	1.05
max.	0.45	0.40	0.90	0.03	0.04	1.20

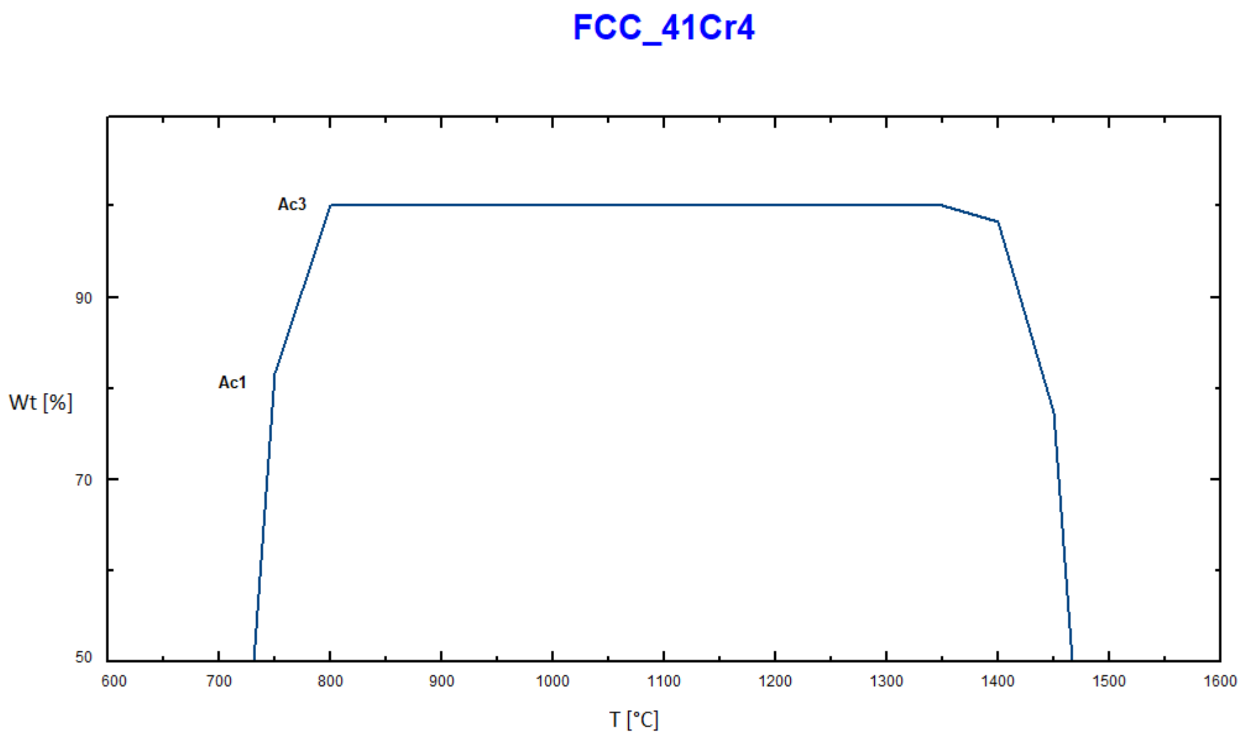

Figure 1 Austenite decomposition graph (created by FactSage) and showing temperatures of Ac3 and Ac1 - steel 41Cr4, composed of average chemical composition from **Table 1**

4. DETERMINATION OF REGRESSION EQUATIONS OF Ac3 AND Ac1

The method of multiple regression analysis was used for the regression equations of the austenite decomposition temperature depending on the chemical composition [11,12]. It is used in cases in which it is necessary to find out certain quantitative variables on one or more other quantitative variables, so-called regressors. It must be determined in advance which variable is independent and which is dependent. The regression method is to determine the dependence of Ac3 and Ac1 on variables using a suitable mathematical model.

4.1. Regression equation of austenite decomposition Ac3 temperature

The basis for creating the regression equation is the determination of the austenite decomposition temperature (Ac1 and Ac3) in the FactSage 8.1 software for 66 combinations of the chemical composition of 41Cr4 steel within the limits defined by the standard. The obtained austenite decomposition temperatures from the software are entered in the Excel table. In individual cases, the Excel 2016 spreadsheet processor, which is part of Microsoft Office, was used for data processing using the multiple regression analysis method. After performing the regression analysis, we get the values that we can substitute into equation (1,2). These regression equations are also the output of regression analysis. A detailed description of the results is given below.

In **Table 2**, the regression results are recorded (already arranged - according to the t Stat value).

Table 2 Ordered regression results (austenite decomposition onset temperature - 41Cr4 steel)

	Coefficients	Mean value error	t Stat	P value
Constant	856.7658146	1.39170839	615.6216496	4.8231E-114
C	-174.6676718	2.359901576	-74.01481216	6.76105E-60
Si	24.13164302	0.370564195	65.12135635	1.17764E-56
Mn	-20.40778728	0.579727471	-35.20238097	2.63583E-41
P	135.0186819	6.317078762	21.37359482	1.8252E-29
S	37.72920461	4.800847145	7.858863961	9.48276E-11
Cr	-5.820929603	0.586102442	-9.931590762	3.32338E-14

First, the statistical significance of the regression model as a whole will be evaluated. The achieved level of significance of the F-test (Significance F) takes the value $2.3862 \cdot 10^{-67}$, which is a much lower value than the selected level of significance α. From this it can be said that the chemical composition has a significant overall effect on the onset temperature of austenite decomposition, which is characterized by the reliability value R (0.99). According to this value, it can be said that the total influence of all elements on the onset temperature of austenite decomposition is 99%. The remaining percentages (1%) express the influence of other aspects, which are not the subject of this work.

Furthermore, the statistical significance of individual regression coefficients will be evaluated. The regression coefficients of all elements acquire lower values in the t-test significance level (P value) than the selected significance level α, therefore they have a statistically significant effect on the solidus temperature.

The influence of statistically significant elements on the temperature of the onset of austenite decomposition decreases according to the column t-Stat, i.e., carbon has the highest effect on the solidus temperature in this case. The regression coefficients of the elements have both negative and positive signs, which means that as the content of a given element increases, the temperature of the onset of austenite decreases or increases. This is because some elements are austenite-forming and others ferrite-forming.

The resulting regression equation for calculating the austenite onset temperature of 41Cr4 steel has the following form

$$T_{Ac_3} = 856.8 - 174.67 \cdot (\%C) + 24.1 \cdot (\%Si) - 20.4 \cdot (\%Mn) + 135.01 \cdot (\%P) + 37.71 \cdot (\%S) - 5.82 \cdot (\%Cr) \quad (1)$$

4.2. Regression equation of austenite decomposition Ac1 temperature

In **Table 3**, the regression results are recorded (already arranged - according to the t Stat value).

Table 3 Ordered regression results (austenite decomposition end temperature - 41Cr4 steel)

	Coefficients	Mean value error	t Stat	P value
Constant	738.723768	2.709318581	272.6603558	3.49E-93
C	6.8590915	4.594155813	1.493003672	0.140765
Si	17.044636	0.721398583	23.6272103	9.07E-32
Mn	14.5533007	1.128588733	-12.89513197	8.18E-19
P	28.5334544	12.29781971	2.320204317	0.023808
S	31.9015675	9.346084619	3.41336172	0.001165
Cr	4.95363044	1.140999256	4.341484368	5.63E-05

First, the statistical significance of the regression model will be evaluated. The achieved level of significance of the F-test (Significance F) takes the value $2.50618 \cdot 10^{-34}$, which is a much lower value than the selected level of significance α. From this it can be said that the chemical composition has a significant overall effect on the onset temperature of austenite decomposition, which is characterized by the reliability value R (0.941). According to this value, it can be said that the total influence of all elements on the solidus temperature is 94.1%. The remaining percentages (5.9%) express the influence of other aspects, which are not the subject of this work.

Furthermore, the statistical significance of individual regression coefficients will be evaluated. The regression coefficients Mn, P, S, Cr, Si acquire lower values in the level of significance of the t-test (P value) than the selected level of significance α, therefore they have a statistically significant effect on the solidus temperature. The coefficients of the C elements do not meet this condition.

The influence of statistically significant elements on the austenite decomposition end temperature decreases according to the t-Stat column, i.e., manganese has the highest effect on the solidus temperature in this case. The regression coefficients of the elements have both negative and positive signs, which means that as the content of a given element increases, the temperature of the onset of austenite decreases or increases. This is because some elements are austenite-forming and others ferrite-forming.

The resulting regression equation for calculating the austenite decomposition end temperature of 41Cr4 steel has the following form:

$$T_{Ac_1} = 738.72 + 6.86 \cdot (\%C) + 17.044 \cdot (\%Si) - 14.55 \cdot (\%Mn) + 28.53 \cdot (\%P) + 31.90 \cdot (\%S) + 4.95 \cdot (\%Cr) \quad (2)$$

5. CONCLUSION

This paper deals with the determination of the decomposition temperature of austenite steel grades (41Cr4) and the design of regression equations for the calculation of these temperatures. The following findings were obtained from the experimental part:

1) The decomposition of austenite takes place in the temperature range Ac3 - Ac1. These temperatures can also be affected by the presence of individual elements in the steel. The austenite-forming elements expand the austenite region and thus reduce the onset and end temperatures of austenite decomposition. Conversely, ferrite-forming elements narrow the austenite region and thus increase the temperature of the beginning and end of austenite decomposition (this is reflected by a negative or positive sign for the regression coefficients of the determined equation).

2) For 41Cr4 steel, the chemical composition has a statistically significant effect on the onset temperature of austenite (Ac3) decomposition of 99% and 1% of Ac3 temperature is influenced by other influences. The regression coefficients of the elements C, Mn, Si, P, S and Cr acquire lower values in the t-test

significance level (P value) than the selected significance level α, therefore they have a statistically significant effect on the Ac3 temperature. The obtained equation (1) has the following form:

$$T_{Ac_3} = 856.8 - 174.67 \cdot (\%C) + 24.1 \cdot (\%Si) - 20.4 \cdot (\%Mn) + 135.01 \cdot (\%P) + 37.71 \cdot (\%S) - 5.82 \cdot (\%Cr)$$

3) For 41Cr4 steel, the chemical composition has a statistically significant effect on the austenite (Ac1) decomposition end temperature of 94.1% and from 5.9% the Ac1 temperature is influenced by other influences. The regression coefficients of the elements Mn, P, S, Cr, Si acquire lower values in the level of significance of the t-test (P value) than the selected level of significance α, therefore they have a statistically significant effect on the temperature Ac1. This condition is not met by the coefficient of element C, and therefore their effect on the temperature Ac1 will not be significant. The obtained equation (2) has the following form:

$$T_{Ac_1} = 738.72 + 6.86 \cdot (\%C) + 17.044 \cdot (\%Si) - 14.55 \cdot (\%Mn) + 28.53 \cdot (\%P) + 31.90 \cdot (\%S) + 4.95 \cdot (\%Cr)$$

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