THE MODELS OF PHASE TRANSFORMATIONS DEFINITION IN THE SOFTWARE DEFORM AND THEIR EFFECT ON THE OUTPUT VALUES FROM THE NUMERICAL SIMULATION OF GEAR THERMAL PROCESSING

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Resume

With the aid of DEFORM® software it is possible to conduct numerical simulation of workpiece phase composition during and upon heat treatment. The computation can be based on either the graphical representation of TTT diagram of the steel in question or one of the mathematical models integrated in the software, the latter being applicable if the required constants are known. The present paper gives an evaluation of differences between results of numerical simulations with various definitions of phase transformation for the heat treatment of a gearwheel and a specially prepared specimen of simple shape. It was found that the preparation of input data in terms of thorough mapping of characteristics of the material is essential.

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1. Introduction

Numerical simulations have become a widespread tool for predicting physical, chemical, biological and other processes and their outcomes. The development of computer technology in 1990s allowed the finite element method (FEM) to be deployed. FEM is a special mathematical technique for finding solutions to differential equations, which delivers higher accuracy than traditional analytical solutions. The complex mathematical apparatus thus becomes available to users without their mastering the highest-level mathematics. This being said, it does not mean that numerical calculations can deliver adequate results without any effort or without the user's profound knowledge of the issue. Today, a number of commercial computer programs are available. Some of them are destined for industrial or pilot plant applications. Their operation is simple and their computations are tailored to one particular manufacturing process. Modifications to process parameters are confined, typically by the choice available from the program's database. These programs, if supplied by renowned producers, make very good tools for technologists in industry. By contrast, the needs of science and development projects are better met by open software. In addition to their own database, such programs contain models which are typically defined by mathematical equations and were developed and verified over the years by prominent researchers. They also permit user data to be entered or new models to be developed. One of such programs is the full version of DEFORM developed by the American company SFTC [1] (DEFORM

offers several variants and modules for simplified simulations). This paper gives a description of simulations of phase transformations and the resulting microstructure of 18CrNiMo7-6 carburizing steel during quenching. The process is used in production of gear wheels for gearboxes of wind turbines.

2. Definition of diffusion-controlled phase transformations

In this section it is necessary to present in details assumptions and procedures of own researchers to such an extent that they can be reproducible. In short papers those information should be given in as short version as possible.

2.1 TTT Diagram

Transformation of austenite to ferrite, pearlite, bainite or martensite is handled by DEFORM on the basis of the diagram of isothermal austenite decomposition (TTT diagram) [2]. Although CCT diagrams (diagrams of anisothermal austenite decomposition) are more frequently and more easily used in practice, there are reasons for employing the TTT diagram [3]. The reasons are given by the logic of the finite element method. The simulated body is split into a large number (hundreds of thousands) of tetrahedral elements and the cooling process is computed for short time steps. Consequently, the phase transformation within a single element over a short time can be considered an isothermal process. A disadvantage to CCT diagrams is the fact that the resulting microstructure is the function of the cooling rate. However, in relation to the finite element method, the cooling rate in a particular element is also affected by the phase transformation taking place. It should be considered whether this fact is accounted for in the computation or whether it is neglected.

In general, the amount of the transformed phase is governed by the temperature, chemical composition and stress in the material [4, 5]. In DEFORM, it is possible to define the diffusion-controlled transformation by a temperature-time table, provided that the phase transformation curve at the start and end of the transformation is known. The dependence on stress may be added as well. Numerical computation requires in all cases the definition of boundary conditions. Where TTT diagrams are to be used, this requirement means that for a particular temperature the start and end of phase transformation should be defined numerically. If diagrams for a particular steel with a given chemical composition are available, the transformation curves between the start and end of the transformation are known within a sufficient temperature range and the effect of stress is neglected, the transformation description is simple. In steels with a carburized layer, the situation is more complicated. A typical TTT diagram for carburizing steel is shown in Fig. 1. It describes En 355 steel (0.20 % C – 0.61 % Mn – 0.23 % Si – 2.00 % Ni – 1.65 % Cr – 0.19 % Mo) with the grain size number 8, austenitized at 800 °C for 30 minutes [6] and shows states prior to carburizing and upon carburizing (the final carbon content was 0.93 %).

The diagram shows the following:

- The curve characterizing the beginning of formation of ferrite (or ferrite-pearlite mixture) is known within a sufficient range of temperatures. However, the diagram does not show the time of the end of the phase transformation for the same temperature range (e.g. at T1 or T2 temperatures in Fig. 1b).

- The content of carbon (the so-called dominant atom in the DEFORM simulation environment) governs the position and shape of the curves, which is why they cannot be constructed with certainty for both carbon concentrations across the entire temperature range (e.g.the bainitic transformation in the non-carburized steel at the T3 temperature shown in Fig. 1b).

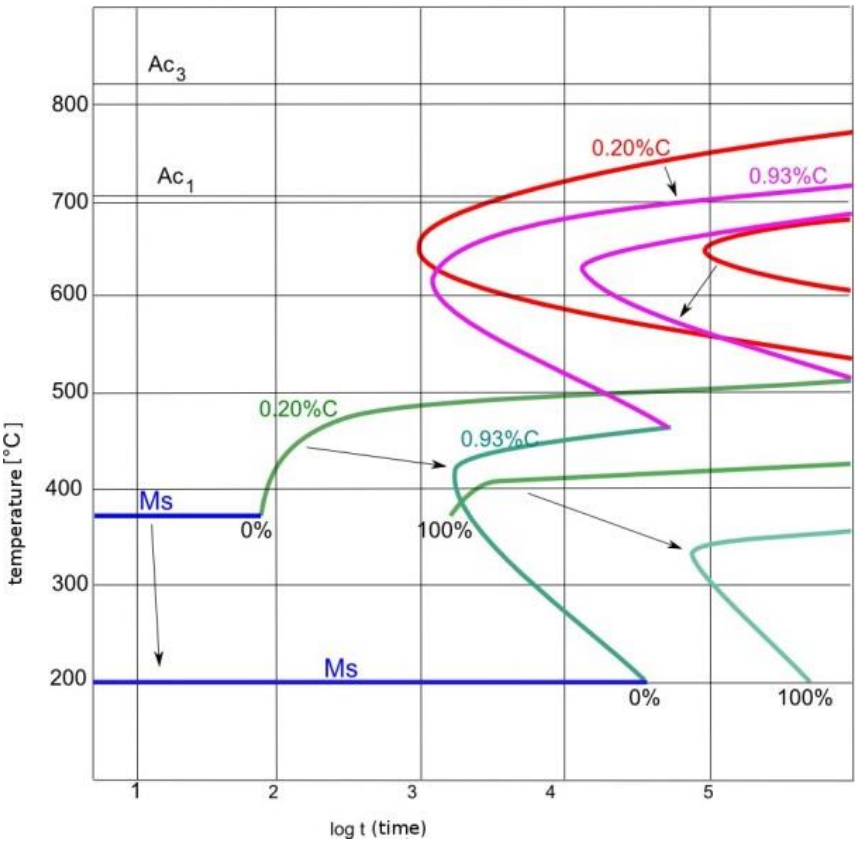

Fig. 1. a) Simplified TTT diagram for En 255 steel.
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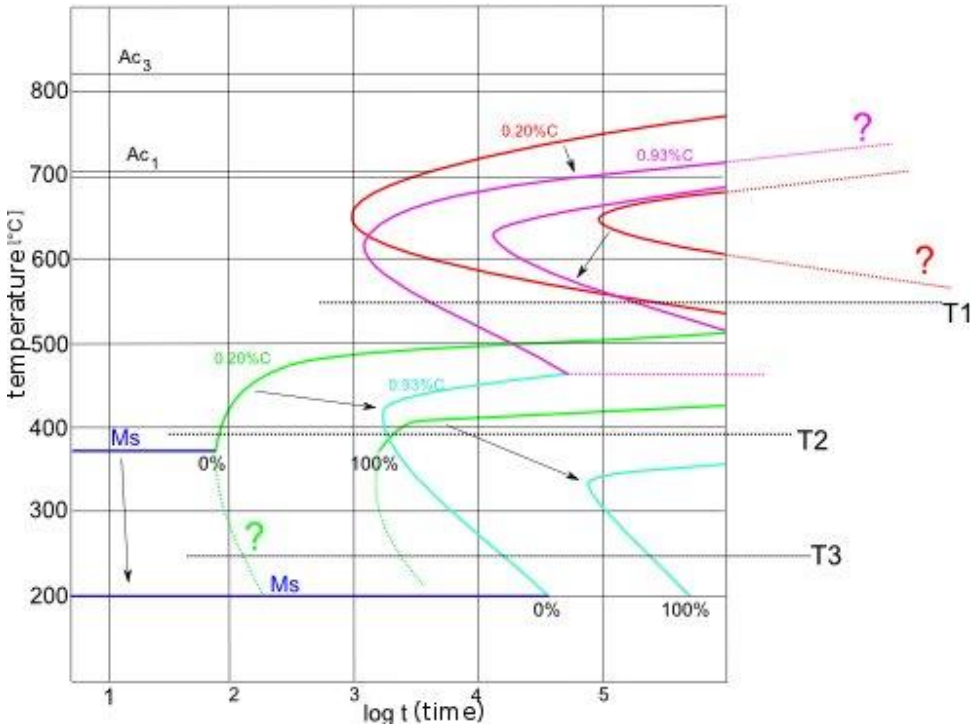

Fig. 1. b) Simplified TTT diagram for En 255 steel.
(full colour version available online)

2.2 *TTT Diagram and Avrami Coefficient*

There is another way to describe diffusion-controlled transformation. It is based on the Avrami equation in the following form

$$\xi = 1 - \exp(-kt^n) \quad (1)$$

where ξ denotes the amount of the newly-formed phase (i.e. the volume fraction where ξ =1 represents the condition with 100 % of the new phase), t denotes time and k and n are constants and n stands for the so-called Avrami coefficient. In this case, DEFORM requires the transformation start curve to be defined in the form of a table. The transformation end is then given by the value of n, the Avrami coefficient. The coefficient can be calculated for a particular temperature, at which the start and end of the phase transformation are known [1].

For each particular phase transformation, this coefficient is then entered as a constant for the entire temperature range of the transformation and regardless of the content of the dominant atom (in this case carbon), although the actual values of the coefficient do vary with temperature. This is another source of inaccuracy or errors. In this case, the effect of stress on transformation was not accounted for in the calculation.

2.3 Diffusion Function Incorporating Effect of Stress [7]

The amount of the newly-formed phase ξ is given by the Avrami equation in the following form:

$$\xi = 1 - \exp(-f_t(T)\, f_s(\sigma_m)\, f_c(C) t^n) \quad (2)$$

where f_t is a function of temperature, f_s depends on the carbon content and accounts for the impact of the mean stress

$$\sigma_m = \sigma_1 + \sigma_2 + \sigma_3, \quad (3)$$

where $\sigma_1, \sigma_2, \sigma_3$ denote principal stresses. The n exponent depends on the transformation. The function f_t can be described by the equation

$$f_T(T) = A_{T1}\left(\frac{T - A_{T2}}{A_{T3}}\right)^{AT4} \cdot \left(\frac{A_{T5} - T}{A_{T6}}\right)^{AT7} \quad (4)$$

where the coefficients A_{T1} through A_{T7} are derived from the 50 % transformation curve in the TTT diagram.

The functions $f_s(\sigma m)$ and $f_c(C)$ describe the dependences on the carbon content and the stress, i.e.:

$$f_s(\sigma m) = \exp(As \cdot \sigma_m) \quad (5)$$

$$f_c(C) = \exp(A_{C1} \cdot (C - A_{C2})) \quad (6)$$

The coefficient A_5 has been determined from the dependence of TTT curves on stress and A_{C1} and A_{C2} were defined by the dependence of the phase transformation on the carbon content. The model indicates that the larger negative number the exponent in equation (2) becomes, the more new phase can be expected to form. This Avrami model of bainitic transformation is available in the DEFORM software database for the SNC 815 material (ISO 15NiCr13). The values of its coefficients are as follows:

A_{T1} = 3.05×10^{-7}, A_{T2} = 150, A_{T3} = 200, A_{T4} = 6, A_{T5} = 550, A_{T6} = 200, A_{T7} = 6, A_S = 0.0030591, A_{C1} = -33.44, A_{C2} = 0.14, n = 4.

3. Diffusionless Phase Transformation: Martensitic Transformation

3.1 Tabular Definition

In DEFORM, it is possible to specify martensitic transformation in the form of a table, provided that the M_s and M50 curves

(curves for martensite start and 50% transformation to martensite, respectively) are known. However, for the simulation to be adequately accurate, these values should be known for various carbon and stress levels.

3.2 Martensitic Transformation Equation

Another description of martensitic transformation relies on the Magee's equation [8] in the following form:

$$\xi_M = 1 - \exp\left(\psi_1 T + \psi_2 (C - C_0) + \psi_{31}\sigma_m + \psi_{32}\bar{\sigma} + \psi_4\right) \quad (7)$$

where ξ_M stands for the amount of martensite, the coefficient ψ_1 accounts for the effect of temperature T, the coefficient ψ_2 describes the effect of the carbon content, the coefficient ψ_{31} relates to the effect of the mean stress σ_m (equation 3) and ψ_{32} covers the impact of the effective stress level, ψ_4 is a constant which, in conjunction with ψ_1, accounts for the effect of temperature. The influence of the stress state is even more significant for the martensitic transformation than it is for the bainitic one.

Tensile stress increases the amount of martensite formed at the given temperature. Compression has an opposite effect, thus stabilising austenite. Transformation to a phase with larger resulting volume relieves tensile stress locally. By contrast, compressive stress within the microstructure hinders the transformation of a phase with smaller volume, i.e. austenite. The presence of tensile mean stress and effective stress raises the *Ms* temperature. *As* a consequence, a small amount of martensite may form even at temperatures around 500 °C in a material containing between 0.2 and 0.5 % carbon. This effect of stress on phase transformation during heat treatment of real-world parts (gearwheels in this particular case) can only be estimated and mapped with the aid of finite element method. Using this technique, mean and effective stress levels are computed for individual elements within the simulated part.

Values of the coefficients needed are available in DEFORM database for SNC 815 steel (15NiCr13): Ψ_1 = 0.016, Ψ_2 = 5.92, Ψ_{31} = -0.0012237, Ψ_{32} = -0.0010303, Ψ_4 = -5.98 and C_0 = 0.14.

4. Simulation of Specimen Quenching

4.1 Simulation Parameters

Where the relationship between input parameters and the outcome is not immediately clear, it is advisable to conduct simulations with various input data and compare the results. It may be found that differences between input quantities are overrated and have marginal effect on the calculation. With this possibility in mind, a quenching simulation was performed. The specimen was a 150×150×200 mm block from 17CrNiMo7-6 material (Tab.1).

The material is used for making gear wheels for gear boxes of wind turbines. The specimen was quenched in oil at 45 °C. The quenching simulation parameters were as follows:

a) Initial temperature of the specimen: 820 °C; oil temperature: 45 °C

b) The carburized layer was split into a 1 mm deep surface layer with the carbon content of 0.55 % and a subsurface layer of the same thickness with the carbon level of 0.45 %C. The carbon content in the base material was 0.17 %.

c) The heat transfer coefficient was adopted from prior simulations. Those simulations were based on curves constructed from data measured in an actual quenching bath at the Wikow s.r.o. company.

Table 1

Chemical composition of 17CrNiMo7-6 steel.

C (%)	Mn (%)	Si (%)	Ni (%)	Cr (%)	Mo(%)	P (%)	S (%)
0,15-0,2	0,4 – 0,6	max.0,4	1,4 – 1,7	1,5 – 1,8	0,25– 0,35	max.0,035	max.0,035

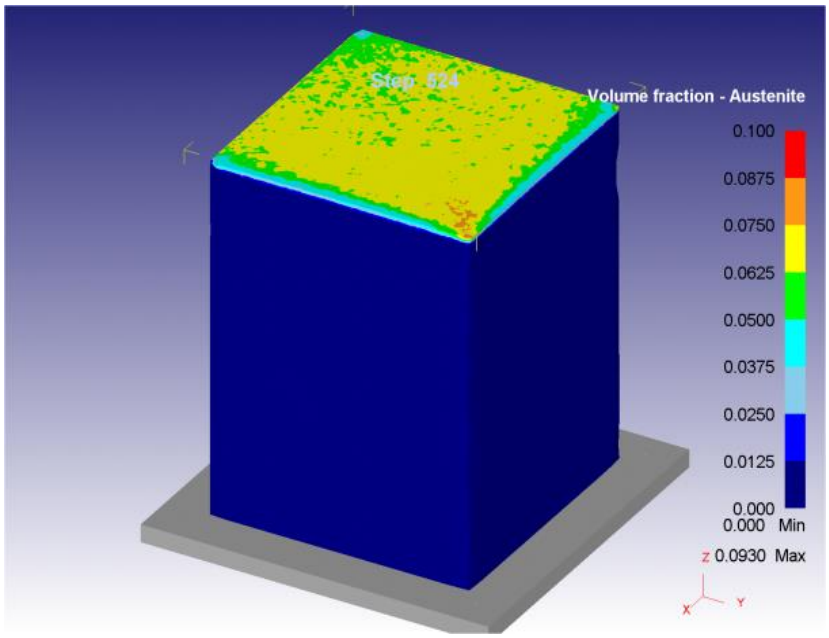

Fig. 2. Untransformed austenite – max. 10 %.
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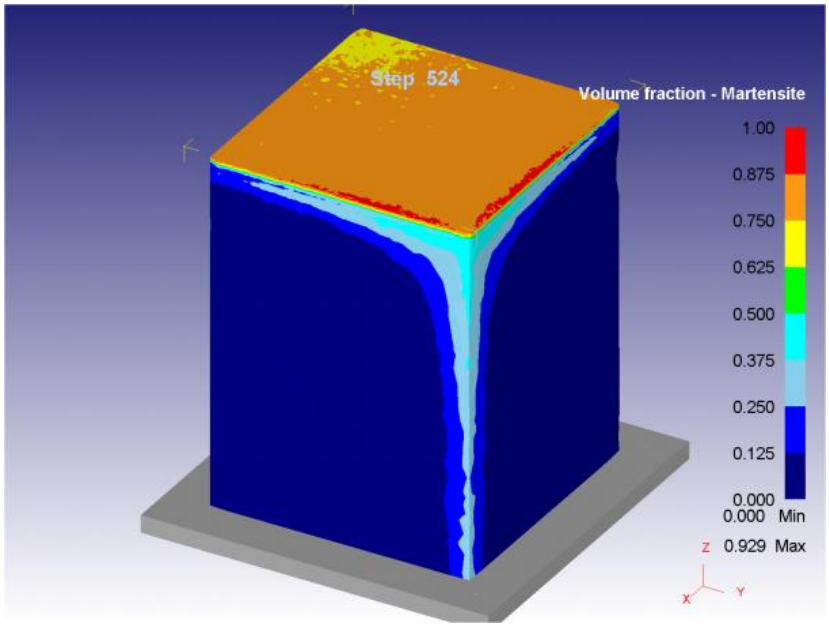

Fig. 3. Martensite after quenching.
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4.2 SNC 815 Material

A quenching simulation was performed for SNC 815 material (15NiCr13). This carburizing steel is similar to the actually used grade. The reason for this substitute was that data for this material is available in the DEFORM database. It includes data on austenite-bainite and austenite-martensite transformations and their dependence on carbon content and internal stress. The dependences are described through Avrami (2) and Magee's equations (7). The austenite-ferrite (or austenite-pearlite) transformation is not included in the model. The phase composition of the specimen upon quenching is shown in Figs. 2 and 3. The carburized layer contains a large amount of untransformed austenite, approx. 7.5 %, and the majority of martensite, 80 %. The interior of the specimen consists of bainite.

4.3 17CrNiMo7-6 Material – Definition a)

Diffusion-controlled phase transformations were defined in the form of a table. The definition was based on the curve for the onset of the phase formation (0.01 % of the new phase) in the TTT diagram for 17CrNiMo7-6 steel prior to carburizing. The data was provided by the gear wheel manufacturer (Wikov s.r.o.). The definition was in part based on data for the similar EN 355 steel upon carburizing (Fig. 1a). In temperature intervals where curves for different chemical compositions are irrelevant, extremely long transformation times were set. The end of the phase transformation was defined in both bases by the calculated Avrami coefficient. A value of n = 2.4 was calculated for the bainitic transformation. The value of the Avrami coefficient for the austenite-ferrite or austenite-pearlite transformation was n = 1.6. No effect of stress is anticipated or accounted for. Martensitic phase transformation was defined by an equation incorporating the impact of stress according to Magee [9]. With this type of the phase transformation description no martensite was found in the resulting microstructure. The carburized layer contained a large amount of untransformed austenite. Virtually no austenite decomposition took place in peripheral regions. In the interior of the specimen, mixture of ferrite and pearlite was found to be present in an amount of less than 20 %.

4.4 17CrNiMo7-6 Material – Definition b)

The austenite-ferrite (austenite-pearlite) and austenite-bainite transformations were specified identically to the case a), as described in section 4.3. Ends of phase transformations were defined using the Avrami coefficient. The austenite-martensite transformation was defined by the M_s (martensite start) and by the M50 (50 % transformation to martensite) curves while taking account of the carbon content only. Effects of stress were not considered in respect of any of the phase transformations. With this type of phase transformation definition, martensite was found predominantly in the edges and corners of the specimen. Central regions of the carburized layer contained less martensite, approx. 25 %. At the surface of the carburized layer, a large amount (up to 35 %) of untransformed austenite was retained. The interior of the specimen contained up to 20 % of the ferrite-pearlite mixture and approximately 80 % bainite, whereas the bainite content in the non-carburized layer below the surface was 100 %.

5. Simulation of Quenching of a Single Tooth on a Gear Wheel of Wind Turbine Gearbox

The phase transformation models were tested in a similar fashion as above by conducting a simulation of quenching of a single tooth with the carburized layer generated by simulation at the depth of 2 mm (Fig. 4).

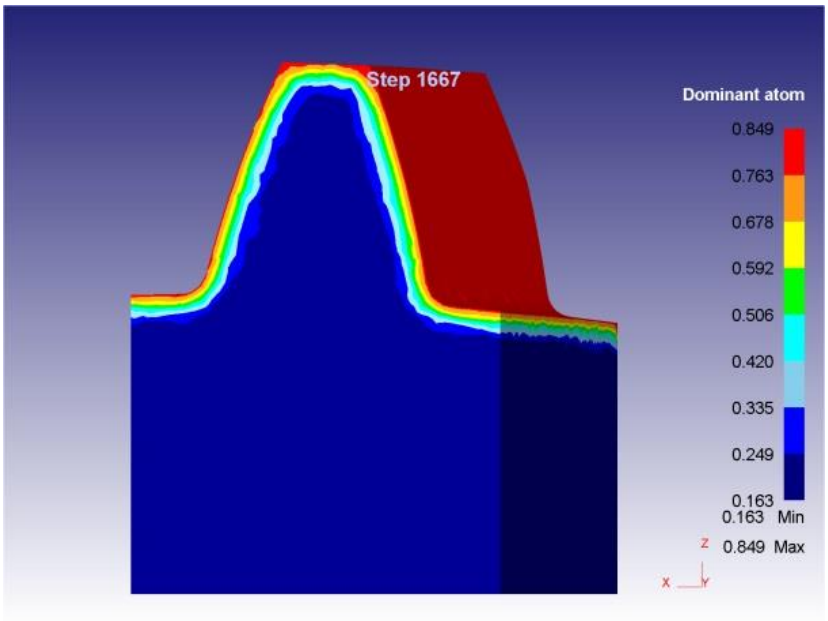

Fig. 4. Carburized layer after simulation.
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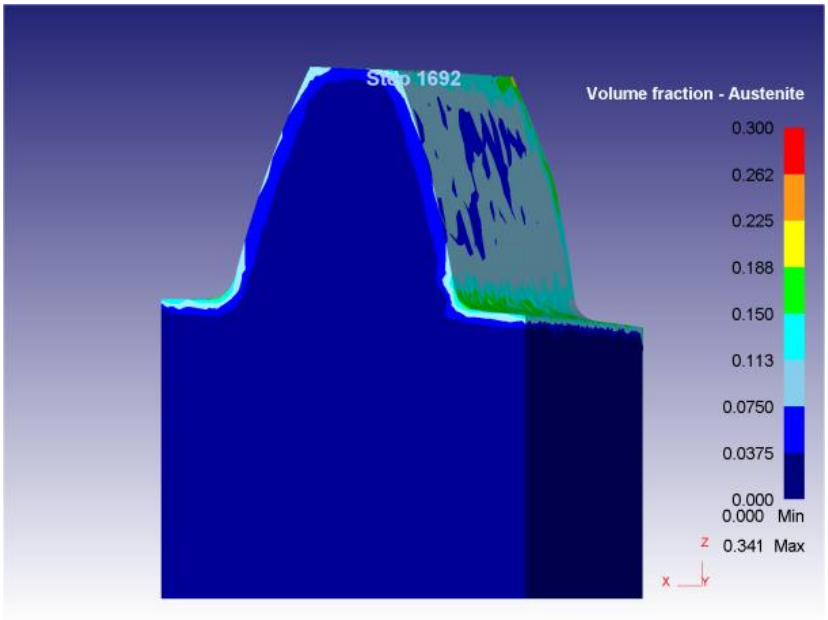

Fig. 5.Untransformed austenite in an amount of no more than 20 % (SNC 815).
(full colour version available online)

5.1 SNC815 Material

Phase transformations were defined identically to the procedure described in section 4.2. Quenching produced typical bainite microstructure. Retained austenite was found on the tooth surface, predominantly in edges on top of the tooth and on the surface of the tooth flank near the tooth base where its amount reaches up to 15 % (Fig. 5). The phase distribution was as anticipated. The carburized layer contained almost 100 % martensite (Fig. 6), whereas the core consisted of bainite. The thickness of the martensite layer is greater at the top of the tooth than near its base, as the latter contains a greater amount of retained austenite. The austenite stabilization is due to the stress state, expressed in terms of the mean and effective stress levels, which prevents phase transformation to martensite (Fig. 7).

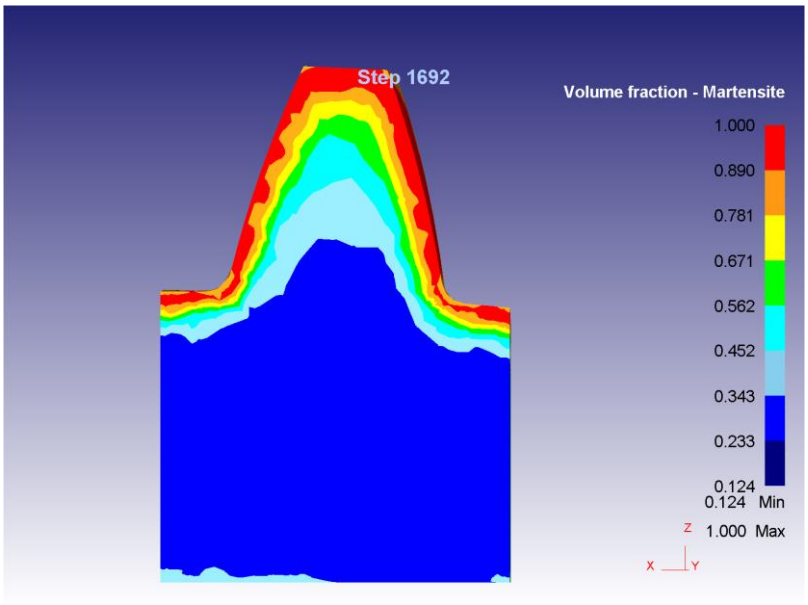

Fig. 6. Martensite (SNC 815).
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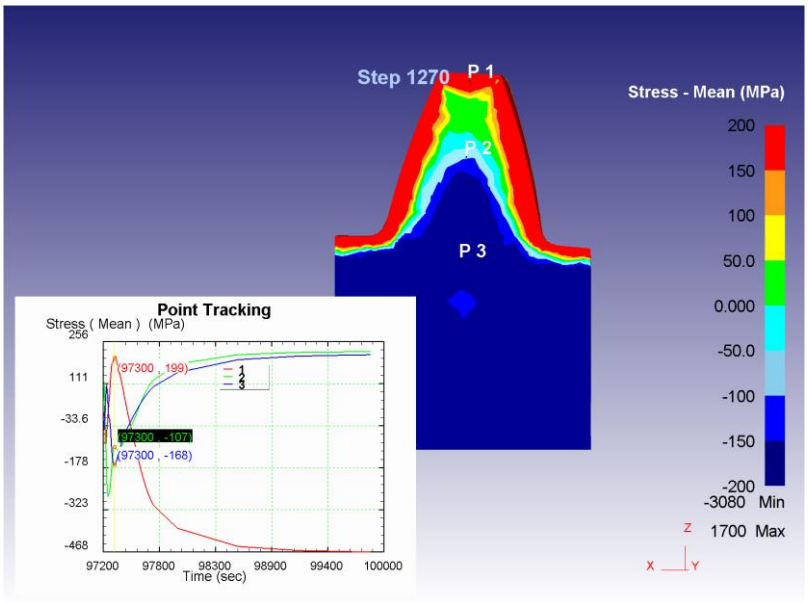

Fig. 7. Mean stress; effect on martensite formation (SNC 815).
(full colour version available online)

5.2 Simulation of Quenching Single Tooth from 17CrNiMo7-6 Material: Definition a)

Phase transformations were specified as in section 4.3. Austenite was effectively stabilized in the carburized layer (Fig. 8). The microstructure also consisted of bainite (Fig. 9). Phase transformation to martensite did not practically occur. The top of the tooth was characterized by prevailing tension stress (Fig. 10), which stabilizes the phase with the smaller unit cell volume, which is austenite in this case. This model is in the best agreement with empirical findings.

5.3 Simulation of Quenching Single Tooth from 17CrNiMo7-6 Material: Definition b)

Materials properties were specified in a manner identical to section 4.4. In this case, too, the content of retained austenite in the carburized layer was high, reaching up to 50 % (Fig. 11). The highest proportion of austenite can be found in the tooth face edges and on the surface at the tooth base. The largest amount of martensite was detected in the top of the tooth, below the carburized layer, reaching up to 80 % fraction, as seen in Fig. 12. The balance consisted of bainite and traces of ferrite.

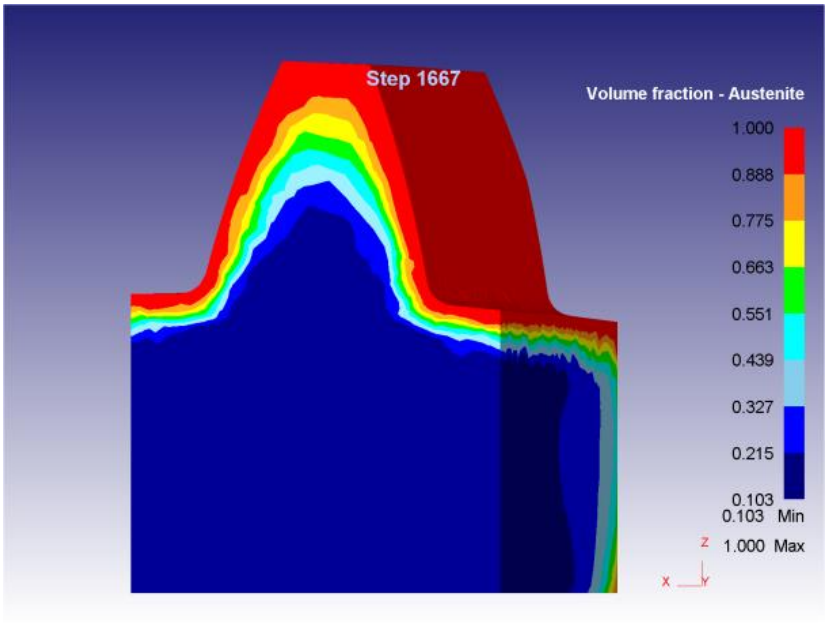

Fig. 8. Untransformed austenite, up to 100 %.
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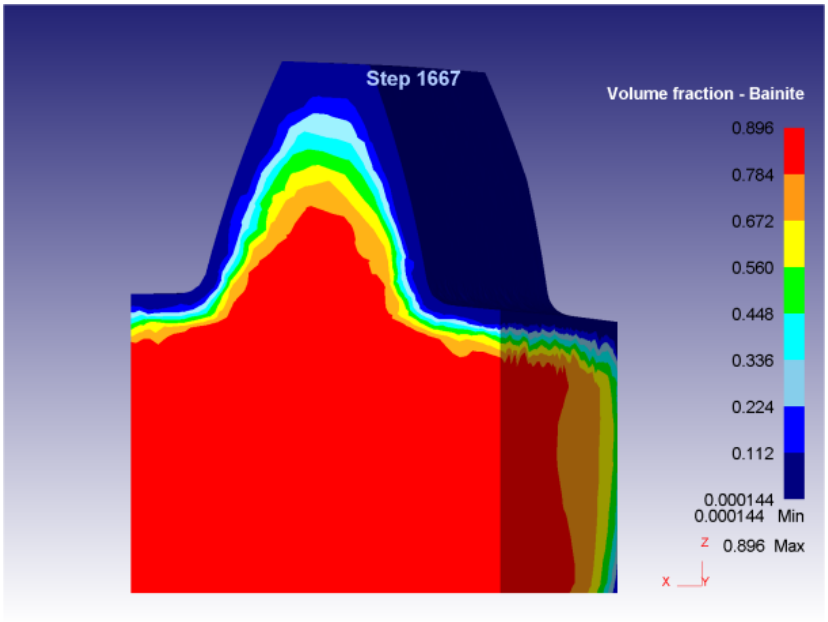

Fig. 9. Bainite.
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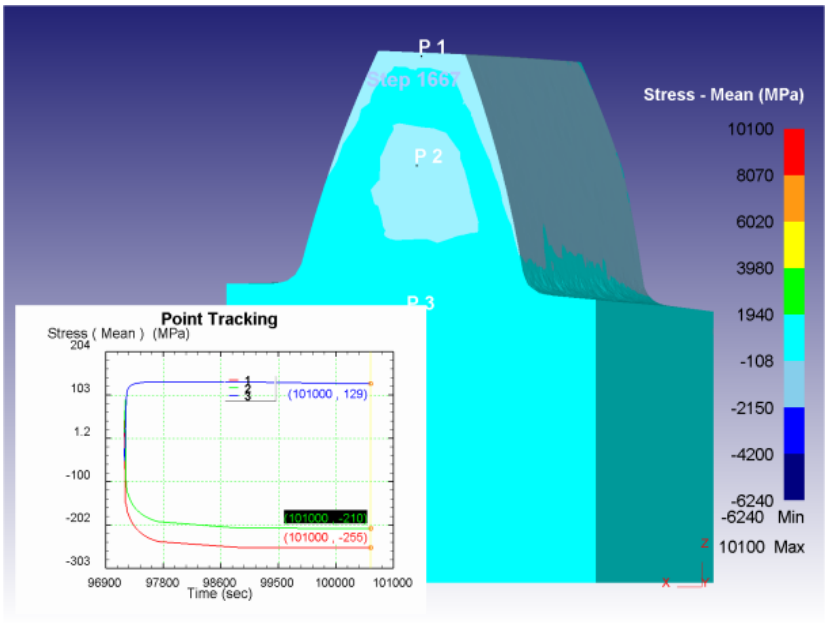

Fig. 10. Mean stress; effect on martensite formation.
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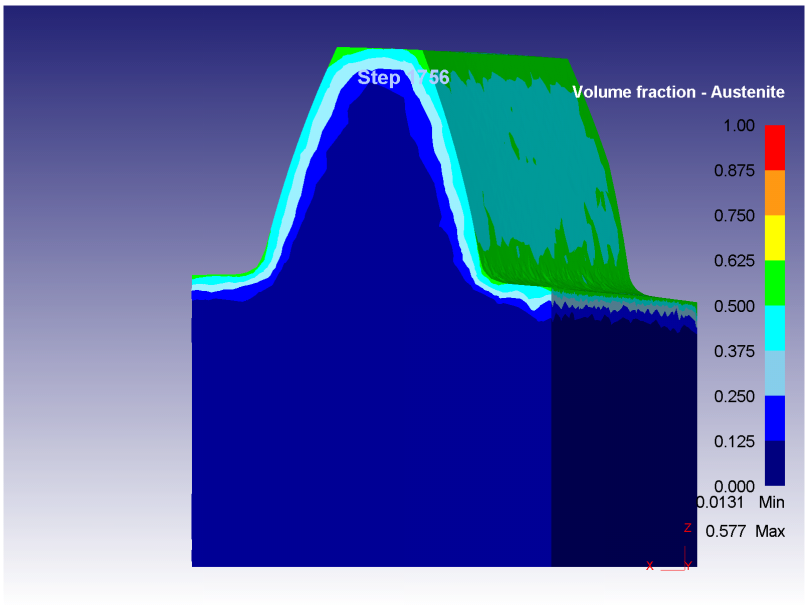

Fig. 11. Untransformed austenite in an amount of up to 50 % on the tooth surface.
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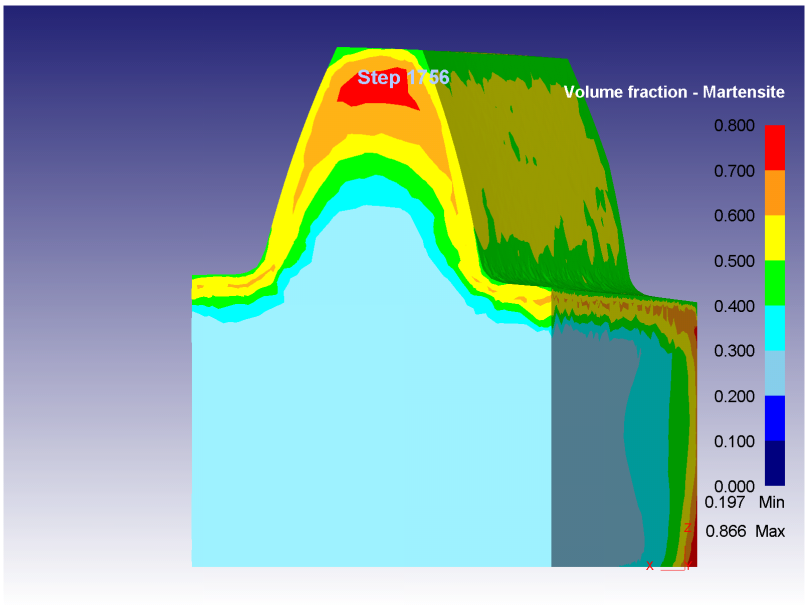

Fig. 12. Martensite after quenching.
(full colour version available online)

6. Conclusion

The study has proven that the resulting microstructure composition is very sensitive to the specification of input data. Empirical experience was best matched by the materials model developed in Japan and included in the DEFORM software database. This was despite the fact that the model described another carburizing steel with a different composition (a higher nickel content, lower chromium level and a negligible amount of molybdenum). When specifying the data, one has to pay great attention to the data preparation. Combining diagrams obtained from literature, adapting them to the DEFORM software requirements and omitting the effects of stress was not successful. Such approach cannot be recommended. For the simulation to be meaningful and valuable for technology development, the following should be done as a rule:

1. Learning about the theoretical background of models integrated in the software. Exploring the data fed into simulations, which also applies to outsourced simulation jobs. Models should be adopted in their entirety. In the present case, the effects of stress on all phase transformations should be incorporated.

2. Devoting adequate resources to testing own materials. The following routes are available:

a) Having TTT diagrams constructed by a certified research facility, taking into account the effects of stress.

b) Fine-tuning a suitable model with respect to findings from metallographic observation. To this end, microstructure composition should be known in several locations of a specimen. In such a case, ordinary light metallography may be as inaccurate and misleading as the simulation itself. A more accurate technique, such as X-ray diffraction, should be applied.

c) Purchasing input data from renowned materials databases [9, 10].

Technologists and development engineers in industry typically do not conduct their own simulations. Whether the simulation contributes to technology development and technology upgrade or becomes a purposeless supplement to research publications and reports depends on the communication and knowledge and experience exchange between industry and the facility where numerical computation is performed. The need for adequate funds should

be borne in mind as well, both for the actual simulation and for preparation of its input data.

Acknowledgment

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References

[1] DEFORM software homepage: http://www.deform.com, accessed 4 Oct 2013.

[2] ASM Handbook: Volume 4: Heat Treating, 10th edition, ASM International, 1991.

[3] D. A. Porter, K. E. Easterling: Phase Transf. in metal Alloys, 2nd edition, CRC Press, 2001.

[4] M. Hillert: Phase Equilibria, Phase Diagrams and Transformations, Cambridge Univ. Press, 1998.

[5] Ge Yu, Y. K. Lai, W. Zhang : Journal of Applied Physics 82(9) (1997) 4270-4276.

[6] Atlas of Isothermal Transformation and Cooling Transformation Diagrams, 1st edition, American Society for Metals, 1977.

[7] C. C. Liv, D.-Y. Ju, K. F. Yao, Z. Liu Z., X.J.Wu: Materials Science and Technology 17(10) (2001) 1229-1237.

[8] C. Magee: Metallurgical Transactions 2(9) (1971) 2419-2430.

[9] http://www.matter.org.uk.

[10] Database of Steel Transformation Diagrams: http://www.steeldata.info.