Simulation of the Transformation Behaviour of Low-Alloyed NiCrMo-Forged Steels - from Data Analysis to Material Model

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Abstract

In this contribution the simulation of transformation behaviour of steels is illustrated with a few examples for low-alloyed NiCrMo steels. Based on extensive data acquisition and analysis a corresponding material model is deduced. The simulation model enables the prediction of microstructure amounts and resulting mechanical properties as a function of steel composition and characteristic temperature-time-sequences for cooling processes after the heat treatment. The model can be used for online and offline applications and for data link operations to numerical simulation systems.

1 Introduction

Low-alloyed NiCrMo-steels belong to the group of high-strength martensitic-bainitic hot working steels. These steels are usually forged and then heat treated.

An important end function of recent materials engineering is the online adjustment of the required material properties. With the steel composition and the technological conditions during the melting process, the secondary metallurgical treatment and during casting, the properties of the steels are only predetermined. The subsequent influence on the forging and the following thermal treatment is relevant for its future use. The design as well as the control of such process chains requires the development of new approaches to characterize the complicated interactions between steel composition, temperature-time-sequences, transformation results, austenite state, cooling conditions, microstructure formation, and mechanical properties. Material models are a probate tool to reveal previously unknown process relationships.

The processes within the material during the forming process have already been discussed on several occasions, e.g. [1-3]. In this contribution we are dealing specifically with the model prediction of the microstructure formation and the resulting properties after heat treatment of the forged parts. With regard to a comprehensive simulation this will provide the opportunity to illustrate a further step in the process chain by linking to the heat treatment module.

Decisive for the mechanical properties is the tempered microstructure pronounced by the transformation and subsequent heat treatment. Due to the difference in wall thickness that is typical for products made from heat resistant NiCrMo-steels, it is necessary to take the temperature distribution in the different cross-sectional areas into consideration. Obtaining a required structure with the cross-section is a property-relevant factor. Therefore, the material-specific setting of temperature and time must be complied with precisely in the critical areas of the forged part. By using FEM-simulation models the temperature sequences in these areas can be illustrated realistically.

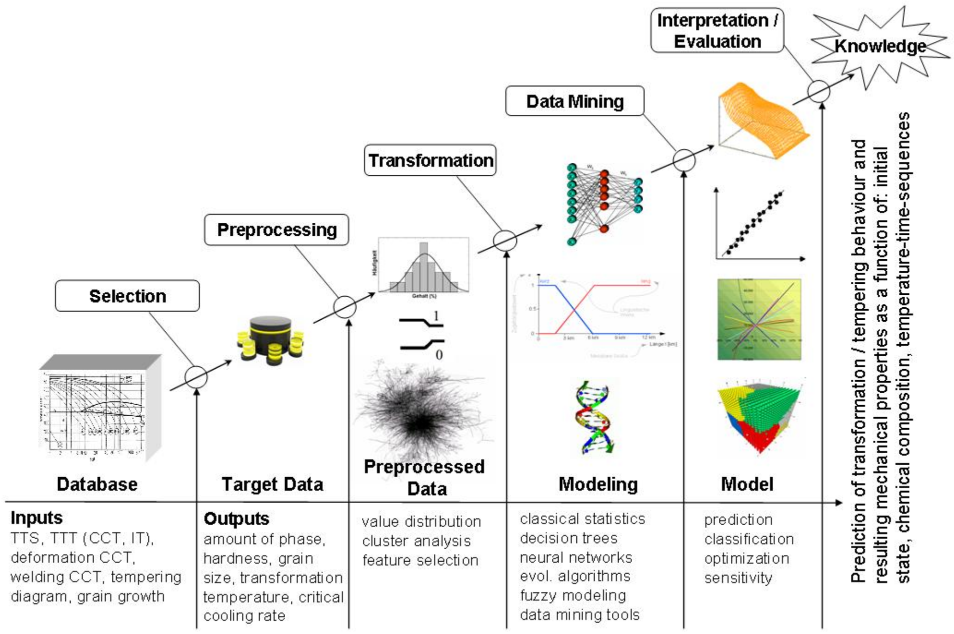

Fig. 1. Steps of data based model development (according to Fayyad inter alia [4])

The correlation between temperature sequence and microstructure formation is described here on the basis of data-based modeling. Fig. 1 clarifies the process steps of this methodology.

2 Parameters to Describe the Transformation Behavior of Steels

In order to ensure an application of databased transformation models that is as comprehensive as possible, material specific parameters must be provided for the transformation behaviour. The efficiency and reliability of the prediction of the models results from the availability of suitable microstructure data and material parameters that are intertwined and parameterized. Data are needed for the modeling that almost completely cover the entire feature space of the system to be modeled. The transformation behaviour of steels can be shown in different ways. Due to the variety of different materials and the nearly unlimited application possibilities, time-temperature-solution (TTS) and time-temperature transformation (TTT) diagrams, tempering or quenching diagrams, as well as grain growth curves (Fig. 2) lend themselves perfectly as data base. Important information sources are the literature (e.g. [5-15]) and the results from experimental studies. All diagrams are valid only for the respectively examined chemical composition and the given marginal conditions.

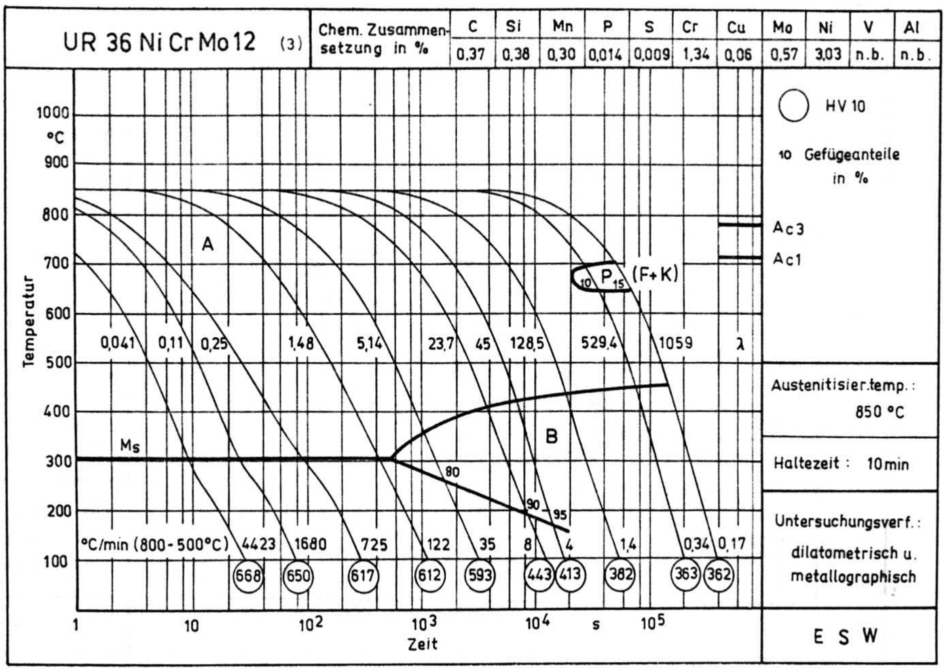

Fig. 2. CCT diagram of steel grade UR36NiCrMo12 [6]

3 Data Analysis

Essential prerequisites for the data analysis are adequate data volume and data quality (measuring accuracies, completeness, etc.). The pre-processing of data is done based on an analytical function apparatus, which makes it possible to reduce the complexity of the data material and to provide relevant information from the data to illustrate cause-effect relationships. The analysis is done on a step by step basis. During a preliminary check of the original data discontinuities in the data sets are eliminated. The data area is then subjected to a statistical analysis.

- Calculation of the correlations,
- Calculation of statistical data (number of discontinuities, span width, standard deviation) and
- Calculation of histograms.

The analysis of the data provides a list with particularities in the value distributions. Data sets that contain outliers will be eliminated.

4 Modeling

Data based models are an efficient instrument to discover the knowledge hidden in data and to utilize it for the application. Such systems use processes of machine learning, such as e.g. statistical analyses, neuronal networks, decision trees and genetic algorithms.

The type of model (prediction, classification or optimization) and the quality of the information available determine the selection of the modeling methods and the type of the mathematical description. Phase transformations of technically relevant steels belong to the complicated technical systems that can only be described inadequately with classically determined models. In order to arrive at acceptable predictions with reasonable expenses we resorted to the method of neuronal networks.

Neuronal networks are typically used for the development of prediction models where the relationships between the input and output data to be analyzed are unknown and defy the knowledge-based physical descriptions. Neuronal networks can be used meaningfully when no analytical model of the analyzed system is available. Neuronal networks are trained with the help of examples (training data) but can also be provided with expert know-how in form of standard rates. The non-linear approximation capability and robust scalability in higher dimensional feature spaces makes neuronal networks a suitable analysis tool that enables better prediction qualities compared to the classic statistical process [16].

The objective of modeling is to show the complex transformation process as well as the tempering behaviour for heat-resistant NiCrMo steels that are subjected to a quenching and tempering process. Not all factors are known quantitatively to a sufficient extent to describe the processes in their relation to the alloy composition. The transformation processes are too complex to describe the entire transformation behaviour with a physical model. Therefore, it is common to examine and model partial processes. A model was developed, among others, to:

- Determine the percentage of the microstructure components ferrite, pearlite, bainite, martensite, and residual austenite in relation to the cooling period $t_{8/5}$,
- Determine the Vickers hardness in relation to the cooling period $t_{8/5}$, and
- Determine the hardness in relation to the quenching temperature.

To configure the neuronal network a suitable network architecture must be defined. This includes the number of hidden layers, the number of neurons per layer, and the transfer functions of the respective layers. In general, the following applies: "as complex as necessary and as simple as possible".

After the configuration of the multilayer perceptrons (MLP), the training will be conducted. The training of the network is interrupted by test phases in order to determine if the required accuracy of approximation has been reached. The decisive information that is provided by the test phase is the error generated by the network.

Once the accuracy of the MLP is acceptable the training phase is concluded. The MLP is capable of making predictions within the limits of the data volume.

This provides the option to estimate the microstructure formation to be expected from different steel compositions within a short period of time. Inhomogeneities as they occur in blooms can also be factored in locally. In addition, the developed MLP can be used to obtain information on the reaction of transformation parameters to a change in the input data.

The boundaries of the input data of the neuronal networks generated for the material group of low-alloyed NiCrMo-steels are shown in Tab. 1.

Tab. 1. Ranges of alloying elements, austenitizing temperatures (T_A), cooling parameters ($t_{8/5}$), and tempering temperature (T_{Anl}) for the low-alloyed NiCrMo steel group

	C [%]	Si [%]	Mn [%]	Cr [%]	Mo [%]	Ni [%]	V [%]	Al [%]	T_A [°C]	$t_{8/5}$ [s]	T_{Anl} [°C]
from	0.18	-	0.15	0.50	0.30	2.2	-	-	820	10	200
to	0.42	0.40	0.70	2.00	0.70	4.0	0.20	0.05	1050	10^5	700

The results of the models is shown in form of quantitative phase diagrams in relation to the $t_{8/5}$ time. Figures 3 and 4 show the microstructure amounts and strength development calculated from the model that are exemplary for two different chemical analyses within the boundaries. The modified carbon and nickel ratios lead to a delay in the bainite start and to an increase in strength under the same cooling conditions.

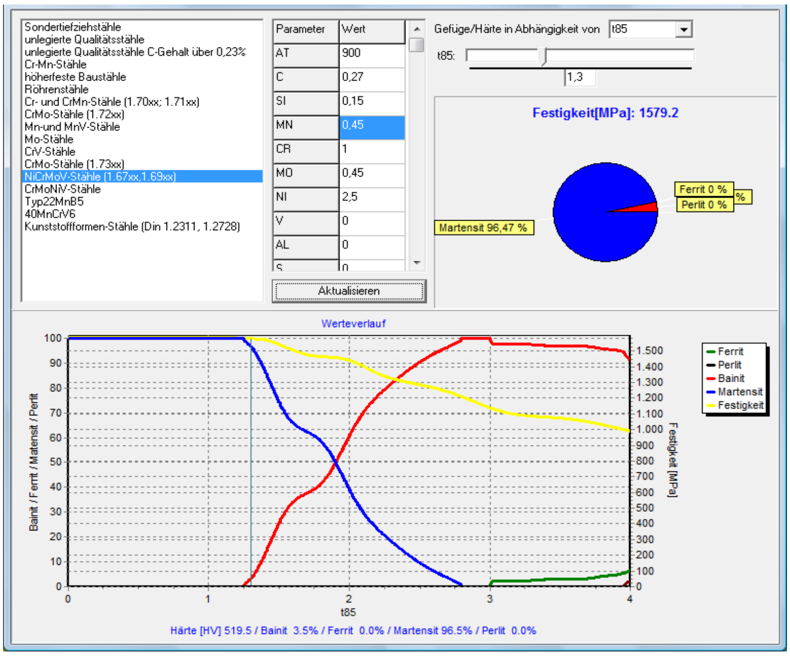

Fig. 3. Quantitative phase diagram of NiCrMo alloyed steel (0.27%C,1%Cr,2.5%Ni)

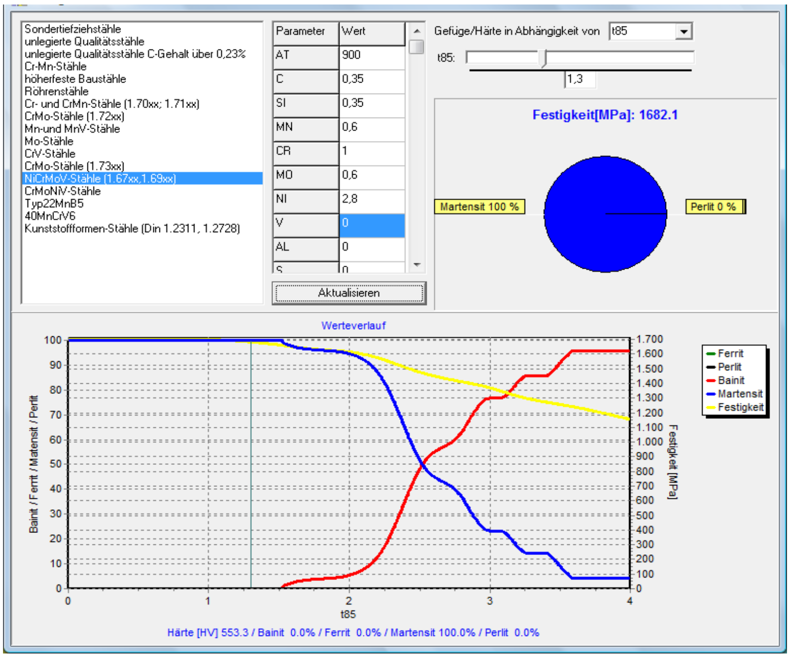

Fig.4. Quantitative phase diagram of NiCrMo alloyed steel (0.35%C,1%Cr,2.8%Ni)

5 Integration of Model Data into the FE-Environment

The developed transformation models were linked to the FEM-simulation program QFORM 3D via standard interfaces.

The heat treatment of a forged fork of the steel grade BS S154 from the aerospace industry was used as an application example (Fig. 5)[1]. The analyzed composition areas are shown in Tab. 2.

Tab. 2. Chemical composition of aerospace standard BS S154

	C [%]	Si [%]	Mn [%]	Cr [%]	Mo [%]	Ni [%]
Minimum	0.27	0.15	0.45	0.50	0.45	2.30
Mean value	0.30	0.25	0.60	0.70	0.50	2.50
Maximum	0.35	0.35	0.70	0.80	0.65	2.80

[1] Courtesy of Mettis Aerospace (UK)

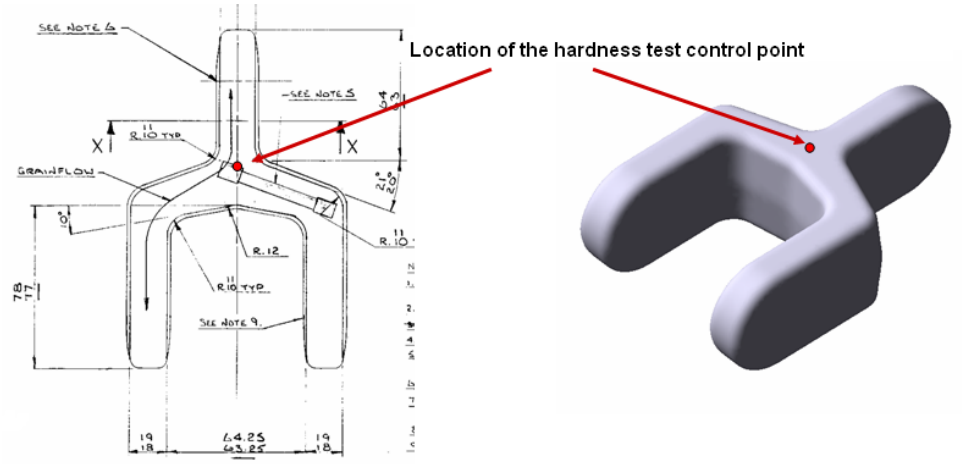

Fig. 5. Drawing and general view of the forged part

The forged fork is annealed for 2-4 hours at 850 °C after the forging, and then cooled in oil, followed by tempering for 3-6 hours at 630 °C/air cooling.

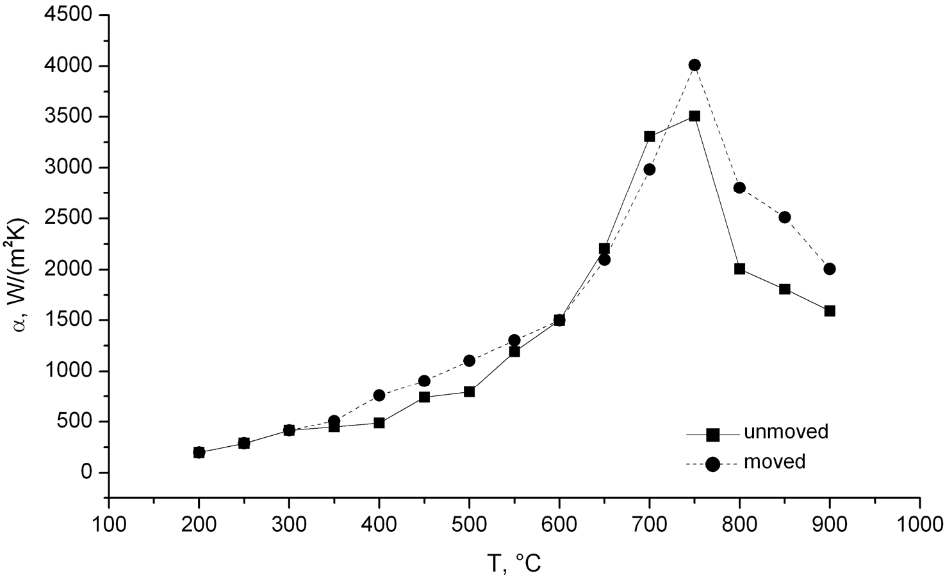

Fig. 6. Heat transfer coefficient vs. surface temperature when quenching in oil

In order to be able to simulate the complete heat treatment the heat transfer coefficients must be determined first. Once the heat transfer coefficients and additional thermo-physical properties are known, such as heat capacity, thermal conductivity, and density, specific cooling processes can be calculated. The temperature dependency of the heat transfer coefficient when quenching in oil is shown in Fig. 6 for the resting and active state.

An FEM-analysis can be carried with the help of the developed models to predict microstructure amounts and hardness for the compositions listed in Tab. 2. Fig. 7 shows examples of simulation results regarding the martensite amount and the surface hardness for the lower (a) and medium (b) content of steel grade BS S154.

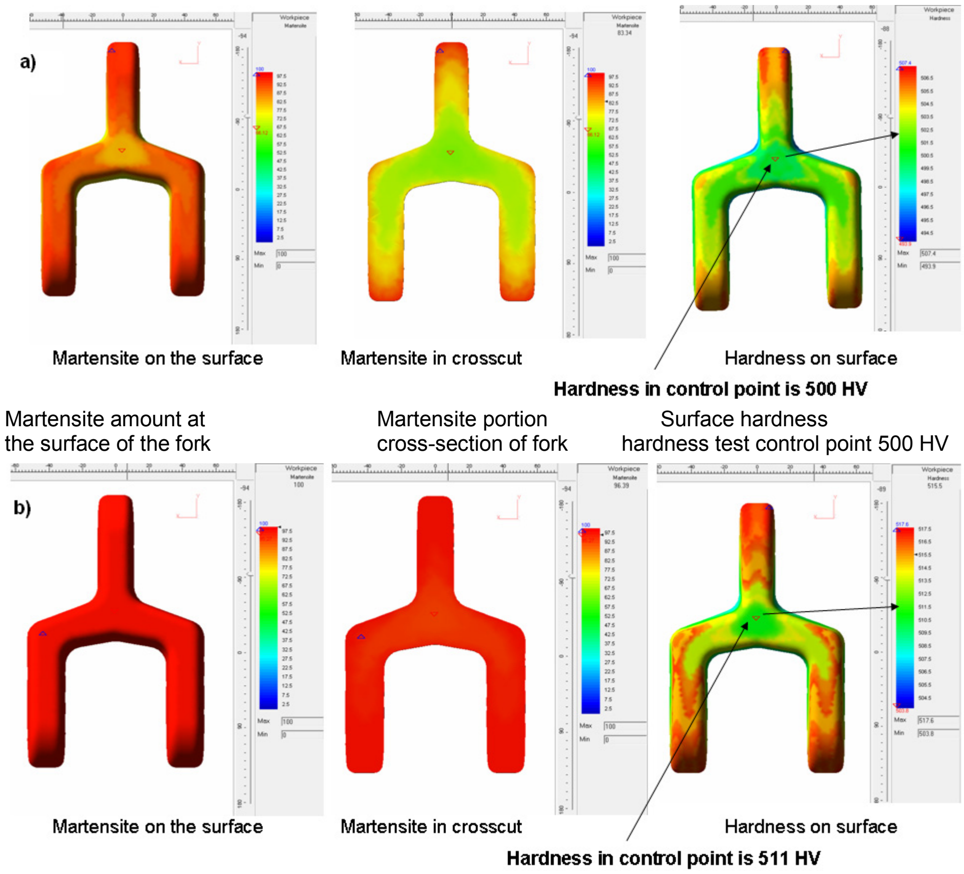

Fig.7. Calculated amount of martensite and hardness on surface for the lower (a) and medium (b) content of alloying elements of steel grade BS S154

The model results are verified based on the hardness test on a critical point of the fork (hardness test control point, see Fig. 7 and Fig. 8). Tab. 3 contains the simulation results for the control point after hardening and the subsequent tempering. An experimental verification resulted in Brinell hardness between 273 and 294 BHN. These hardness data correspond to tensile strengths (Rm) between 925 and 990 N/mm². A comparison of the simulated hardness data with the experimentally determined ones show that the developed models provide for an acceptable prediction quality.

Tab. 3. Simulation results in the control point after quenching (H) and tempering (A)

Alloy content	$Martensite_H$ [%]	$Hardness_H$ [HV]	Rm_H [N/mm²]	$Hardness_A$ [HV]	Rm_A [N/mm²]	$Hardness_A$ [BHN]
Maximum	100	547	1810	340	1080	323
Mean value	95	511	1665	295	950	280
Minimum	66	500	1630	290	920	276

The result proved that the simulation of the complex relationships between component geometry, steel composition and heat treatment parameters can be done with near practice software solutions. Consequently, the simulation contributes to an optimization of the heat treatment processes in addition to a better understanding of the microstructure and property changes that are taking place.

6 Conclusion and Outlook

The introduced models on the basis of neuronal networks contain inherent knowledge on the transformation behaviour of the examined steel group and provide information on the microstructure formation and mechanical properties. They support the realization of complex relationships between the steel composition, the austenitization and cooling conditions, and the mechanical properties resulting from the microstructure amounts.

The simulation results will be used to optimize the thermal treatment. Since the influence of the chemical composition on the transformation behaviour and the resulting properties becomes accessible immediately with the help of these models, the optimization of the steel composition can be done strategically with regard to a desired microstructure property combination.

The approach to describe the transformation behaviour of NiCrMo steels introduced here is already being used for additional steel groups. In addition to the models for predicting microstructure amounts and hardness data, there are also data based models available for the prediction of transformation temperatures (A_{C3}, A_{C1}, A_{r3}, A_{r1}, M_S, B_S), critical cooling speeds in the respective microstructure phases as well as the beginning and end of isothermal transformations.

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