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# Simulation of Heat Treatment of Carburization and Nitrocementation of 16MnCr5 Steel

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## Abstract

Simulation is used today in many contexts, such as simulating technology to tune or optimize performance, safety engineering, testing, training, education, and entertainment. In some industries, simulations are commonly used, but in heat treatment this is rather an exception. The paper compares the simulation of carburization and nitrocementation of 16MnCr5 steel with a practical application. The aim was to determine the applicability of chemical heat treatment simulation. We were looking for an answer to the question: to what extent can we rely on the technological design of heat treatment? The software designed the heat treatment technology. He drew the technological process of chemical-thermal treatment of 16MnCr5 steel. The thickness of the cementite layer was 1 mm and the nitrocementation 1.2 mm. Changes in mechanical properties were observed. Cementing, nitrocementing, hardness, microhardness, metallography, and spectral analysis were practically performed. This article describes the benefits of simulation, speed and accuracy of the process. The only difference was in determining the carbon potential. The simulation confirmed the practical use and its contribution in the technological process.

**Keywords:** Cementation, Nitrocementation, Heat treatment, Simulation

## 1. Introduction

Surface treatment of materials together with chemical-thermal treatment are widely used in automotive, aerospace and general engineering. During the processes of carburization and nitriding, the surface properties of the material are intentionally changed. The aim is to achieve the higher hardness and wear resistance of components while maintaining high flexibility of the core, which resists dynamic stress [1]. With the right processing procedure, the steel acquires the required properties and can subsequently be used in construction in various areas of production. Only those elements that form solid solutions with iron or intermediate phases have the ability of the steel to saturate the surface. To create saturation, resp. The chemical process occurs at a certain temperature over a certain period. Thermochemical processing processes are of great practical importance because they increase the physical and mechanical properties and thus improve the overall quality of the material [1, 2].

According to Mallener et al., the effect of heat treatment on the quality of the part is 20-40% [2]. They represent their effects such as furnace type, furnace storage, cooling uniformity, atmosphere used, etc. The remaining 50-60% is the choice of material such as chemical composition, structure, and geometry. Heat treatment changes the mechanical properties and creates a new structure of the material [3]. As 16MnCr5 steel is widely used in the automotive and aircraft industries, it is still under investigation. The technologist must consider energy savings and the impact on the environment. The subject of research is not only the cooling environment, but also the kiln atmosphere. For example, R. Altraszkiewicz et al. [1] investigate the effect of helium and hydrogen as a substitute for nitrogen. 16MnCr5 steel has a wide range of possibilities in this regard [1, 2].

Currently, there is a high trend of renovation of these technologies using software simulation programs, which are used to optimize chemical-thermal treatment processes. The software can define the most efficient process for steel based on its specifications, which include partial characteristics such as chemical composition, design geometry, cooling conditions or hardened and tempered conditions for nitriding and nitrocementation processes [4]. The simulation can calculate the hardness of carbon or nitrogen profiles for a given depth of the surface layer, the sequence of process curves of the profile curve of the expected carbon and nitrogen distribution.

The article describes the course of cementation and nitrocementation of 16MnCr5 steel in the simulation process and compares the results with practical application [3-5].

# 2. Experimental procedure

Two cylindrical samples, Ø 20 mm, were made for the experiment. A different chemical-thermal treatment temperature was defined for each of these samples and based on this, the structures were compared, the core hardness and the surface hardness after the chemical-thermal treatment were measured. The simulation program verified the sample processing technology.

## 2.1. Simulation software

HT-Tools simulation software is a multi-purpose program used to design the optimization of heat treatment processes. It is designed for the process of cementation, carbonitriding, nitriding and nitrocementation. The simulation will reduce the lead time for process development and replace time-consuming evaluations and trials. HT-Tools analyses the entered data and models the carbon, nitrogen, and hardness content.

For nitriding and nitrocementation, the software manufactures models in accordance with AMS Recommendations 2759 / 10A and 2759 / 12A.

This software contains a material database that can be populated with steels of various chemical compositions. Depending on the alloying elements in the steel, it also calculates alloying factors and solubility limits compared to precipitation from carbides and nitrides. Simulation of various alternatives by changing parameters allows the user to quickly evaluate the procedure to achieve optimal results.

It also determines the thickness and composition of the surface layer, the diffusion layer, the total diffusion depth, the hardness profile with tolerances, the percentage of carbon, the surface carbon and nitrogen content, the carbide or nitride limit and the soot limits [5, 6, 7].

The composition of the steel is formed and adjusted by setting the temperature in the heating, holding and cooling phases, the atmosphere of the cementing furnace - specification of carbon or nitrogen potentials, soot limits, carbide limits and surface carbon content. The parameters of thermo-chemical processing were presented by the software based on thermodynamic calculations.

## 2.2. Carburization

The software created a simulation of the carburization of the sample by analysing the entered data. The diagram (Fig. 1) shows that the red curve describes the course of the carburization temperature of the steel, the orange curve indicates the carbon potential, the brown curve indicates the percentage of carbon on the surface.

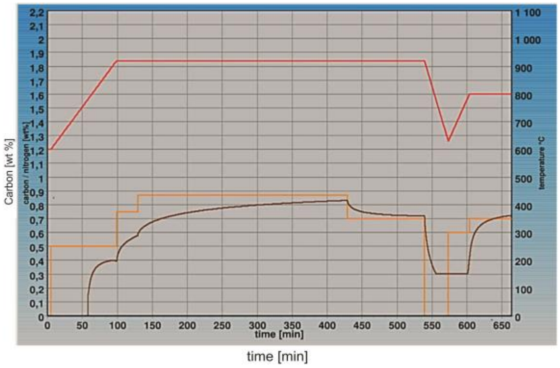

Fig. 1. Simulation of carburization

The processing takes place above the temperature AC3, i. at temperatures of 910-930 ° C, because only austenite can form a solid solution with carbon - to absorb carbon into its crystal lattice in either a liquid, gaseous or solid environment. The carbon content should not exceed 0.8%, which is the concentration of eutectoids, so there would be large embrittlement of the carbonized layer [5-8].

The first experimental sample was cemented to a thickness of 0.8-1.0 mm. The determined technological procedure is shown in Tab. 1, the chemical-thermal treatment process is shown in a diagram (Fig. 2) from a furnace chamber furnace. This diagram describes the violet curve of the carbon potential as a function of the change in temperature and time of cementation. Oil cooling.

Table 1.
Technological process

| **Operation** | **Temperature [°C]** | **Time [h:m]** | **carbon potential Cp [%]** |
|---|---|---|---|
| Pre-heating | 610 | 00:05 | - |
| Heating | 920 | 01:30 | 0.50 |
| Dwell | 920 | 05:10 | 0.87 |
| Dwell | 920 | 01:55 | 0.70 |
| Cooling | 720 | 00:40 | 0.70 |
| Heating | 800 | 00:20 | - |
| Dwell | 800 | 01:10 | 0.60 |
| Cooling | 20 | 03:00 | 0.70 |

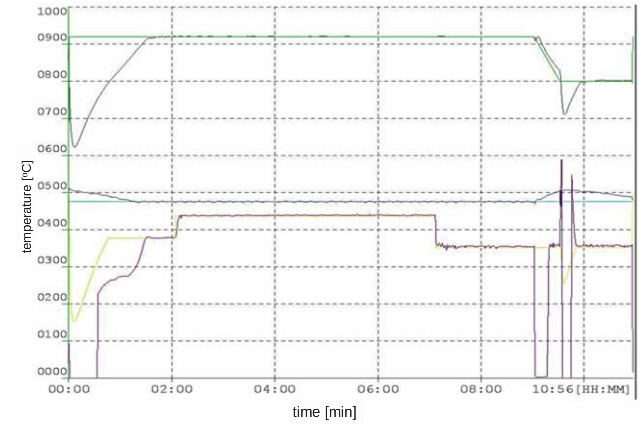

Fig. 2. Diagram of carburization

The hardness was determined on an automatic Duramin A300D microhardness tester. It was measured from the hardened surface to the core. The course is shown in tab.2 and fig. 3. the average value of unheated steel is 232 HV (22.18 HRC), after heat treatment the steel has an average surface hardness of 698 HV (60 HRC) and an average core hardness of 298 HV, which is according to the ASTM 31.3 HRC hardness conversion.

Table 2.
Hardness from surface to core

| Point [no.] | Distance [mm] | Hardness [HV 1] |
|---|---|---|
| 1 | 0.10 | 717 |
| 2 | 0.20 | 711 |
| 3 | 0.60 | 646 |
| 4 | 0.70 | 600 |
| 5 | 0.80 | 552 |
| 6 | 0.90 | 534 |
| 7 | 1.00 | 487 |
| 8 | 1.10 | 429 |
| 9 | 1.20 | 411 |
| 10 | 1.30 | 396 |
| 11 | 1.40 | 358 |

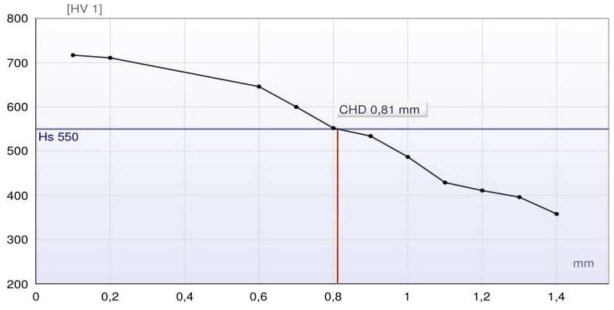

Fig. 3. The course of hardness from the surface to the core of the carburizing sample

The samples were evaluated on an Olympus GX 51 metallographic confocal inverted microscope. The surface layer and the slightly heat-affected core of the material were always analysed (Fig. 4). There is a significant difference in structure between the surface and the core of the material. The surface carbonized layer is formed by a bainitic structure containing perlite and residual austenite. Bainite is not present in the core (Fig. 5), the structure is coarse-grained, pearlitic with a slight content of residual austenite. The fine grain and the even distribution of the carbonized layer guarantee an improvement in the mechanical properties of the material, such as e.g., increased hardness and improved machinability.

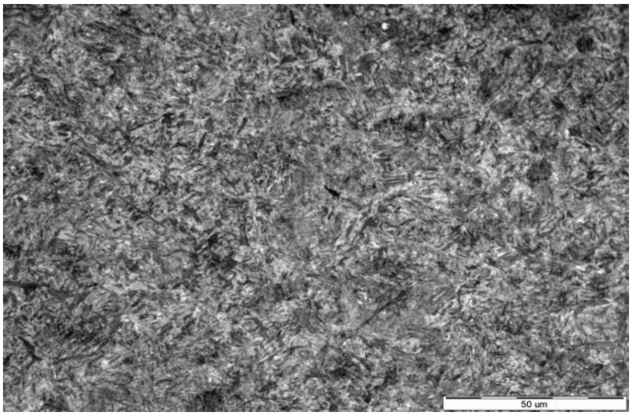

Fig. 4. The surface structure of carburizing sample 16MnCr5, etching. Nital (3%), vol. 200x

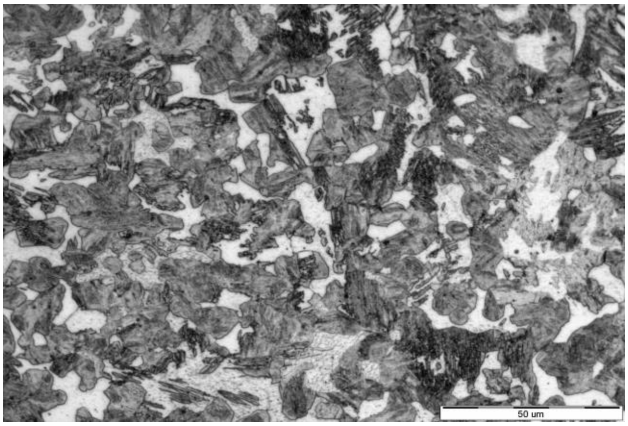

Fig. 5. Sample core structure - 16MnCr5, etching. Nital (3%), vol. 200x

## 2.3. Nitrocementing

The second sample underwent a nitrocementation process with hardening to a thickness of 0.8-1.2 mm. Fig. 6 presents a simulation of heat treatment, the red curve describes the nitrocementation temperature of the steel, the orange curve indicates the carbon potential, the brown curve indicates the percentage of carbon on the surface, the pale green curve indicates the nitrogen potential and the dark green curve indicates the percentage of nitrogen on the surface.

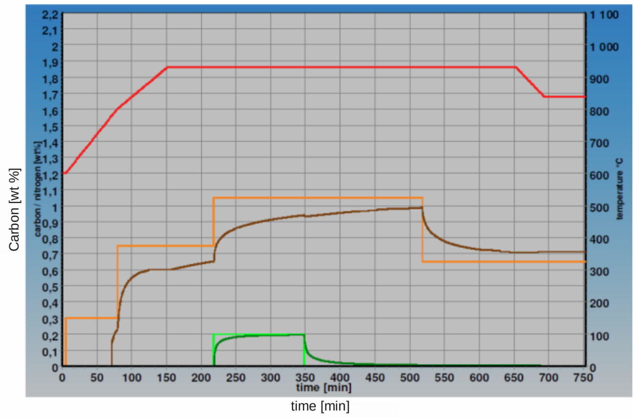

Fig. 6. Nitrocementation simulation

The aim of nitrocementing is to form a surface layer containing 0.8 - 1.0% C and approximately 0.3% N, while the properties of the core do not change. The properties of the surface layer are conditioned by the predominant carbon, nitrogen has an effect on the acceleration of saturation. This process has the same course as the saturation process during cementation, but the advantage of nitrocementation is the lower risk of growth of unwanted austenitic grain. Nitrogen diffusion also accelerates carbon diffusion. Nitrogen increases the solubility of carbon in the surface layer and thus increases the growth rate of the nitrocementite layer [8-11]. The growth rate of the nitrocementite layer at 860 ° C is approximately equal to the growth rate of the cementation layer at 920 ° C. The determined technological procedure is presented by Tab. 3.

Table 3.
Technological process

| **Operation** | **Temperature [°C]** | **Time [h:m]** | **carbon potential Cp [%]** | **nitrogen potential Np [%]** |
|---|---|---|---|---|
| Pre-heating | 600 | 00:05 | - | - |
| Heating | 930 | 01:45 | 0.75 | - |
| Dwell | 930 | 01:00 | 0.75 | - |
| Dwell | 930 | 02:10 | 1.05 | 0.20 |
| Dwell | 930 | 02:15 | 0.65 | - |
| Cooling | 840 | 00:30 | 0.65 | - |
| Dwell | 840 | 01:10 | 0.65 | - |
| Cooling | 20 | 03:30 | 0.65 | - |

The process of chemical-thermal treatment is shown in the diagram - Fig. 7, from a multi-purpose furnace. This diagram describes the violet curve of the carbon potential as a function of the change in temperature and time of cementation heat treatment.

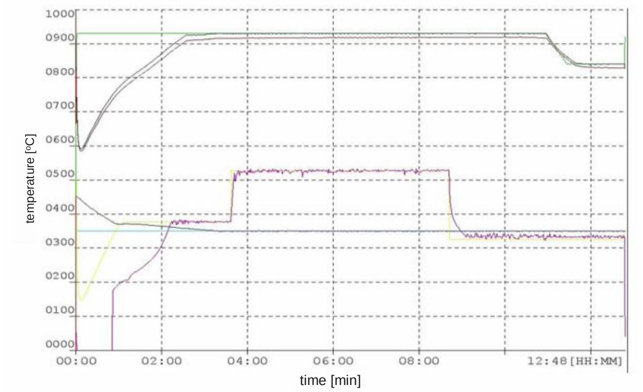

Fig. 7. Diagram of nitrocementation

The average value of unheated steel is 248 HV (22 HRC), after heat treatment the steel has an average surface hardness of 722 HV (61 HRC) and an average core hardness of 363 HV( 37 HRC). The measurement process is shown in tab. 4. and fig.8, where the hardness decreases from the surface to the core of the sample.

Table 4.
Hardness from surface to core

| **Point [no.]** | **Distance [mm]** | **Hardness [HV 1]** |
|---|---|---|
| 1 | 0.10 | 724 |
| 2 | 0.20 | 722 |
| 3 | 0.60 | 695 |
| 4 | 0.70 | 658 |
| 5 | 0.80 | 643 |
| 6 | 0.90 | 612 |
| 7 | 1.00 | 583 |
| 8 | 1.10 | 549 |
| 9 | 1.20 | 516 |
| 10 | 1.30 | 506 |
| 11 | 1.40 | 480 |

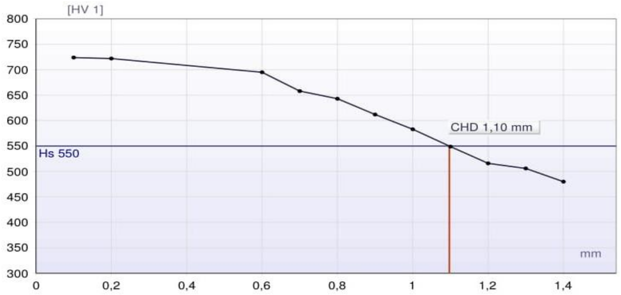

Fig. 8. The course of hardness from the surface to the core of the nitrocementing sample

The microhardness measurement was used to evaluate the mechanical properties of the small dimensions of the samples and the thin layer of the surface, to identify the individual structural phases in the metallography. It is an advantageous way of researching the mechanical properties of a small volume of material with minimal destruction, so it is also suitable for the research of final products.

The surface structure (fig.9) of the sample is located in the area of existence of austenite. By adding carbon to the surface layer, we can reduce the austenitic region to 770 ° C. The sample became rapidly turbid above $A_1$, whereby austenite was diffuselessly changed to martensite at a critical cooling rate, and a martensitic structure with a hardness of 61 HRC was obtained. Despite the fact that the steel became sharply turbid, we can see white triangular segments, which are referred to as the percentage of residual austenite. The martensitic structure of the surface consists of coarse martensite together with a larger proportion of residual austenite [11, 12]. This proportion of residual austenite was caused by the different rate and time of cooling of the sample. The core is formed by bainite and residual austenite (fig.10).

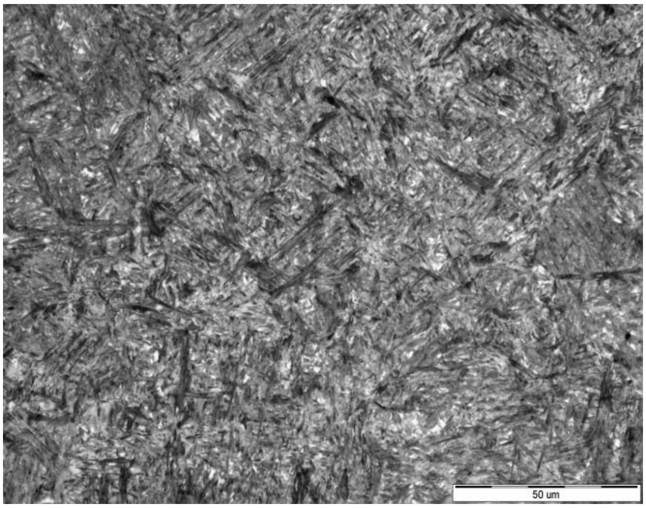

Fig. 9. The surface structure of nitrocementing sample 16MnCr5, etching. Nital (3%), vol. 200x

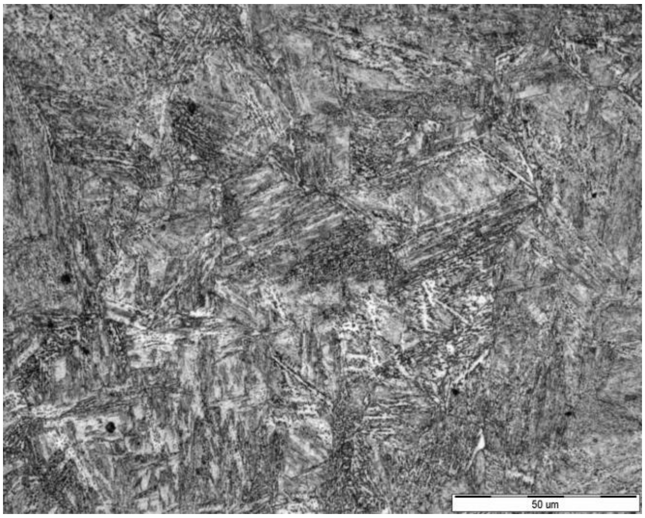

Fig. 10. Sample core structure of nitrocementing - 16MnCr5, etching. Nital (3%), vol. 200x

## 3. Results and discussion

Spectral analysis of the material was also one of the control tests. The carbon and manganese contents were monitored. Monitoring the % carbon content is important in terms of chemical heat treatment. The manganese content was monitored due to a possible change in chemical composition after heat treatment of 16MnCr5 steel. Different carbon content in the test material can result in an unfavourable distribution of internal stresses, which increase with volume changes at the surface and in the core. This affects the choice of curing temperature. The work determined that the oil-cooled to 20 ° C.

Table 5.
Chemical composition

| **The Element** | **Non heat treatment [%]** | **The sample of carburization [%]** | **The sample of nitro cementation [%]** |
|---|---|---|---|
| C | 0.15 | 0.688 | 0.603 |
| Si | 0.189 | 0.2 | 0.199 |
| Mn | 1.139 | 0.823 | 0.667 |
| Cu | 0.053 | 0.048 | 0.051 |
| Al | 0.017 | 0.016 | 0.017 |
| Cr | 1.14 | 0.797 | 0.647 |
| Mo | 0.046 | 0.042 | 0.04 |
| Ni | 0.047 | 0.045 | 0.046 |
| Co | 0.014 | 0.008 | 0.007 |

Spectral analysis was performed on a Belec compact port spectrometer. The results of the spectral analysis show an increase in the carbon content in the surface layer of individual samples. The manganese content of the material was significantly affected by the thermal process. After heat treatment, there was also a decrease in chromium, molybdenum, nickel, cobalt and an increase in carbon, nitrogen, silicon, and iron.

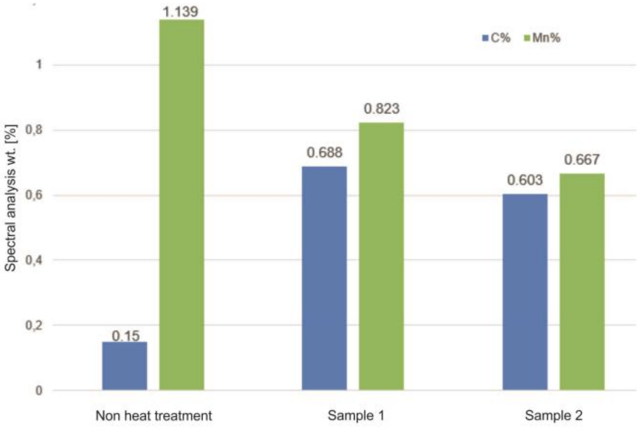

Fig. 11. C (blue) and Mn (green) content [%] before and after chemical-thermal treatment

The implementation of software simulations evaluated various changes in the parameters of chemical-thermal treatment operations in comparison with the practical results.

There were discrepancies between the software and the actual results from the furnace schemes, specifically in determining the carbon potential in the atmosphere. We assume that the difference in carbon potential between the simulation and the actual value was due to the influence of the furnace atmosphere. Although the calculation of the simulation is very accurate, in practice there are always smaller differences.

The use of simulation and the possibility of adjusting parameters is very practical and reduces the need for costly testing.

## 4. Conclusions

The work uses the simulation program HT Tools to determine the parameters of heat treatment of 16MnCr5 samples. The simulations were verified in practice. The course in the furnace and the design of the simulation of heat treatment of 16MnCr5 steel are almost identical.

Carburization took place at temperatures of 910-930 °C. The thickness of the carbon coating is 0.8-1.0 mm. The hardness of the carbon coating is 717 HV. A bainitic structure was formed.

Nitrocementing coating is 0.8-1.2 mm and was formed at 930 ° C. The achieved hardness is 724 HV. The structure is martensite. The formation of martensite can be explained by the longer time of the sample in the furnace. Nitrocementation lasted 100 minutes. longer than cementation.

Cementation and nitrocementing changed the mechanical properties - the surface hardness of the part increased threefold, and the core remained relatively soft. The hardness of the surface between the samples themselves reaches an approximate value, visibly the samples differ in the composition of microstructures.

## Acknowledgements

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