Simulation-based optimization of the local material state in the field of cyclically highly stressed case hardened construction details with notch effect

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Summary
Steel components have different construction details, such as cross holes and rounded shaft shoulders in the case of bending loaded components. By an external loading the shape of the construction details causes local extreme values of the multiaxial stress state (notch effect). Under cyclic loading they cause crack initiation and the component fails.

The fatigue strength of cyclically loaded components can be considerably increased by the heat treatment case hardening. The shape of the construction detail has a significant influence on the sub-processes of the case hardening. This relates to the carbon diffusion during carburizing and the local heat transfer during quenching. As a result, after the case hardening process the local material state is often not optimal in terms of phase composition and residual stresses.

To solve the problem, a heat treatment simulation based on a Finite Element method is connected with high order methods to solve optimization problems. Under consideration of the component loading condition, it is possible to adapt technological parameters of the case hardening process to the form of the construction detail, whereby it was possible to increase the fatigue strength and to improve the efficiency of the case hardening process itself.

Key Words
Heat Treatment, Case Hardening, Simulation, Optimization, Fatigue Strength, Construction Detail, Notch Effect.

Introduction
Steel components have different function-related construction details. Typical details are for example cross holes and rounded shaft shoulders in the case of bending loaded components or cross and stepped bores in high pressure loaded components. Due to external loading of the component their shape cause local extreme values of the multiaxial stress state (notch effect). Under cyclic loading they cause crack initiation and the component fails. Therefore, the basic objective is to increase the strength of the components material. The fatigue strength of cyclically loaded components can be considerably increased by the thermal-chemical heat treatment case hardening [3, 4]. Normally such influences will not be taken into consideration to determine technological parameters of case hardening such as, for example, carbon level, carburizing times and quenching media characteristics. Furthermore, relevant targets of case hardening such as surface hardness, carbon and case depth are usually defined and measured in easily accessible locations of the component.

The heat treatment simulation has become more and more important for the optimal design of heat treatment processes and for the optimization of the component’s properties. If the heat treatment simulation is coupled with modern mathematical solution procedures to solve optimization problems, expanded possibilities are offered to adjust relevant parameters of the case hardening process to the special requirements of construction details [5].
Simulation and Optimization of case hardening processes

As illustrated in Fig. 1 the simulation model of the case hardening process consists of three subsequent coupled analyses and different interactions among them [6]: A carbon diffusion analysis to determine the carbon field in the component, a coupled quench thermal and phase transformation analysis to determine local histories of temperature and phase fields and finally a residual stress analysis. Each analysis is represented by partial or ordinary differential equations that are solved numerically by using the Finite Element Method (FEM) [7, 8]. All the material parameters needed in the simulation have to be defined phase and temperature dependent with respect to the chemical composition of the case hardening steel and the varying carbon content in the surface layer of the component.

The process parameters will be varied within user-defined fields and the designs which are so generated are analyzed by the FE-solver SYSWELD. For each output parameter, such as carbon content, core hardness, but also degree of utilization due to external loading, a so-called Metamodel of Optimal Prognosis (MOP) [11] based on polynomial or Moving Least Squares approximations is created. The adequacy of the approximation can be assessed by the Coefficient of prognosis (COP). Based on this coefficient an assessment variable will be defined to estimate the importance of a single input parameter on the corresponding output parameter [12]. In this way it is possible to identify the most important parameters.

For the numerical optimization of case hardening processes, it was first necessary to couple a finite element program for the analysis of heat treatment processes with a solver for optimization problems. Here, the commercially available programs SYSWELD [9] and optiSLang [10] have been used. The coupling is essentially based on an implementation in the batch mode of SYSWELD and an automated text-based output of all relevant results of the FE nodes with the help of the SIL script language. The component stress state has to be taken into consideration and it was therefore of the SIL script language. The component stress state is subsequently subjected to a sensitivity analysis.

Finally a response-surface optimization of the case hardening process is carried out by using the Meta-model of Optimal Prognosis. Within the optimization the technological parameters of the case hardening process are adapted to objective functions, which are minimized or maximized under consideration of constraints. Possible optimization goals are in addition to the hardness or the composition of the microstructure in certain areas of the component also the increase of the component strength and the improved efficiency of the case hardening process. The determined optimum, the so-called best design, is verified with a single call of the FE-solver SYSWELD.

In order to improve the endurance limit of case hardened components the multiaxial stress state due to external loading is assessed according to the widely used Dang-Van criterion [13, 14] in terms of shear stress amplitude $\tau$ and hydrostatic pressure $p$, Figure 3.

![Figure 1: Simulation of case hardening processes, acc. to [6](#)

![Figure 2: Optimization of case hardening processes](#)

![Figure 3: Dang-Van criterion](#)
The fatigue limit in fully reversed torsion \( \tau_w \) and the sensitivity to hydrostatic pressure \( \alpha \) are defined in dependency of the local hardness after tempering. In the case of the shear fatigue limit the former austenite grain size is additionally taken into account as an internal defect [15, 16]. The residual stresses are considered as additional hydrostatic stresses \( p_{\text{res}} \). A Dang Van equivalent stress is then given by:

\[
\sigma_{\text{eq}, \text{DV}} = \tau(t) + \alpha \cdot (p(t) + p_{\text{res}})
\]  

(1)

The resulting optimization criterion is defined on the basis of the maximum degree of utilization as objective function:

\[
f = \max[\eta] = \max \left[ \frac{\sigma_{\text{eq}, \text{DV}}}{\tau_w} \right] \quad \text{component} \rightarrow \text{MIN}
\]  

(2)

This criterion has to be evaluated over the whole component. In the case of the FE method the objective function is evaluated on the FE nodes. The objective function takes into account gradient effects from the stress state (external loading) and the material state.

Example: Optimization of the case hardening process of a shaft with cross hole

The Figure 4 shows the geometry shaft with cross hole made of case hardening steel 18CrNiMo7-6, Table 1. The shaft is loaded under cyclic bending load. The technical parameters of the standard case hardening process (gas carburizing / oil quenching) are given in Table 2.

Figure 4. Shaft geometry with cross-hole in mm

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Si</th>
<th>S</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.17</td>
<td>0.58</td>
<td>1.56</td>
<td>1.43</td>
<td>0.26</td>
<td>0.24</td>
<td>0.031</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Table 1. Chemical composition of the case hardening steel 18CrNiMo7-6 in wt.%

| Carburizing: Temperature \( T_C \) = 960 °C |
| --- | --- | --- | --- | --- |
| Carbon potential | 1 | 2 | 3 | Soaking on quenching temperature |
| C [%] | 0.97 | 1.18 | 0.73 | 0.73 |
| t [min] | 20 | 180 | 30 | 60 min |

| Quenching: Temperature \( T_Q \) = 860 °C; Medium Oil, 60 °C |
| --- | --- | --- |
| Tempering: Temperature \( T_T \) = 160 °C, 2 h |

Table 2. Technical parameters of the case hardening process

As a result of the FE analysis of the bending load, Figure 5 shows a plot of the equivalent stress for a bending moment of 264 Nm. The high stressed volume which leads to the failure of the component is on the cross hole surface near the corner.

Figure 5. Shaft with cross-hole, high component volume (red) due to external bending load

The simulation of the case hardening process according to Table 2 was carried out using the material data base from SYSWELD and the research project C.A.S.H. [17]. The Figures 7 to 9 are showing representative results from the different analyses, Figure 1.

Figure 6. Standard carburizing process, carbon concentration in wt.%
Figure 7. Standard carburizing process, dimensionless volume fraction retained austenite

Figure 8. Standard carburizing process, Vickers hardness after tempering

Figure 9. Standard carburizing process, axial residual stresses in MPa

Figure 10. Overview sensitivity analysis and optimization of the case hardening process of the shaft with cross hole. For the comparability with the standard carburizing process (Table 2), the carburizing and quenching temperature have not been varied within the sensitivity analysis. The optimization was carried out on the basis of the Metamodel Optimal Prognosis. The constraints defined allow the limitation of carburizing time (C1), reaching a minimum carburizing depth (C2) and a limitation of the maximum carbon content in the high stressed volume (C3).

The Figure 10 shows an overview sensitivity analysis and optimization of the case hardening process of the shaft with cross hole. For the comparability with the standard carburizing process (Table 2), the carburizing and quenching temperature have not been varied within the sensitivity analysis. The optimization was carried out on the basis of the Metamodel Optimal Prognosis. The constraints defined allow the limitation of carburizing time (C1), reaching a minimum carburizing depth (C2) and a limitation of the maximum carbon content in the high stressed volume (C3).

Sensitivity Analysis

Parameters
- Carbon potential and carburizing times
  \( CP_1, CP_2, CP_3, t_{CP1}, t_{CP2}, t_{CP3} \)
- Carburizing temperature: \( T_C = 960 ^\circ C \)
- Quenching temperature: \( T_Q = 860 ^\circ C \)
- Advanced Latin Hypercube Sampling (ALHS) \[18\]

50 Samples

Responses
- max. carbon concentration on area \( B \)
- carbon concentration cross hole, distance 0.8mm

Single-Objective Optimization, based on MOP

Criterion, on FE nodes \( i \)
\[ f = \eta^{(i)} = \frac{\sigma^{(i)}}{\tau_0^{(i)}} \rightarrow \text{MIN} \]

Constraints
- \( C1: \sum_{i} t_{CP1} + t_{CP2} + t_{CP3} \leq 6000s \)
- \( C2: c_x(0.8\text{mm})_{\text{max}} \leq 0.25 \text{ Ma.-%C} \)
- \( C3: \text{max. } c_x \leq 0.70 \text{ Ma.-%C} \)

Optimization method
- Nonlinear Programming by Quadratic Lagrangian (NLPLQ approach) \[18\]

As a result of the sensitivity analysis, the Figure 11 shows the importance of the input parameters of the
case hardening process on the Dang Van degree of utilization. The largest variance of the model is described by the carbon potential 3. Furthermore the overall quality of the approximation is good (COP = 90%). In addition, Figure 12 shows the response surface of the Meta Model of the Dang Van degree of utilization in the subspace of the most important parameters.

In Figure 13 the optimized technological process parameters, which result from the Metamodel Optimal Prognosis are presented. These parameters have been verified with a single solver call of SYSWELD. According to the Standard case hardening process the representative results are shown in Figures 14 to 17. Due to the optimizing process it was possible to adjust the carbon content. This results in a considerably reduced retained austenite content. Compared to the Standard case hardening process the hardness and the compressive residual stresses in the high stressed volume are improved, whereby the fatigue strength is increased. The determined Dang Van degree of utilization of the optimized case hardening process of the shaft with bending load 1.23.
Table 3 presents a comparison of results of the investigated variants. The surface hardness and core hardness obtained with both investigation variants differ only slightly and meet industrial minimum requirements. Alongside with the fatigue strength increase it was possible thanks to the optimization to limit the total carburization time and the maximal carbon potential. This process efficiency improvement leads also to a reduction of the case hardening depth in the cross hole area. The reduction does not mean a lower fatigue strength of the component.

### Conclusion

During the case hardening process the shape of the construction details has a significant influence on the achievable local material state in terms of phase composition and residual stresses. By the coupling of FE based simulation of the heat treatment process and of mathematical methods for optimization problems, it is possible to adapt technological parameters of the case hardening process to the form and the loading condition of the construction detail. In the presented case hardening example of a bending loaded shaft with cross hole it was possible to increase the fatigue strength and to improve the efficiency of the process itself.

### Abbreviations

#### Text:
- $p$ – Hydrostatic pressure
- $p_{RS}$ – Hydrostatic pressure due to residual stresses
- $\sigma_{DV}$ – Dang Van equivalent stress
- $\tau$ – Shear stress amplitude
- $\sigma_{W}$ – Fatigue limit in fully reversed torsion
- $\sigma_{DV}$ – Sensitivity to hydrostatic pressure
- $\eta$ – Degree of utilization
- $t$ – Time
- $C_C$ – Carbon concentration
- $CP$ – Carbon potential
- $t_{CP}$ – Carburizing time
- $T_C$ – Carburizing temperature
- $T_Q$ – Quenching temperature

#### Criterium | Standard case hardening process (SP) | Optimized case hardening process (OP) | Difference
---|---|---|---
max. carbon concentration | 0.84 wt.% | 0.66 wt.% | - 21 %
max. retained austenite content | 0.35 | 0.23 | - 34 %
max. hardness | 632 HV 1 | 680 HV 1 | + 8 %
axial residual stresses | - 199.5 MPa | - 267.8 MPa | + 34 %
Surface hardness, diameter $d = 30 \text{ mm}$ | 684 HV 1 | 685 HV 1 | -
CHD, GH = 550 HV, diameter $d = 30 \text{ mm}$ | 1.02 mm | 0.74 mm | - 28 %
Core hardness | 431 HV 1 | 436 HV 1 | -
max. Dang Van utilization rate | 1.32 | 1.23 | - 9 %
max. carbon potential | 1.18 % C | 1.06 % C | - 11 %
Total process time | 290 min | 140 min | - 52 %
Figure 16. Optimized carburizing process, Vickers carburization time and the maximal carbon potential. was possible thanks to the optimization to limit the total investigated variants. The surface hardness and core hardening example of a bending loaded shaft with itself.

- During the case hardening process the shape of the construction detail has a significant influence on the state in the field of cyclically highly stressed case hardened construction details with notch effect from the Research Association for Steel Application (FOSTA, Forschungsvereinigung Stahlanwendung e. V.). The research project (IGF-Nr. 17779 BR, 01.05.2013 - 30.06.2015) is supported by the Federal Ministry of Economic Affairs and Energy within the German Federation of Industrial Research Associations (AiF - Arbeitsgemeinschaft industrieller Forschungsvereinigungen „Otto von Guericke“ e. V.), which is based on a resolution of the German Parliament. We would like to thank all funding organizations as well as the Project Support Committee led by Mr. Dipl.-Ing. Rainer Salomon (FOSTA).

Acknowledgments

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References


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<th>Carbon Potential CP</th>
<th>Surface Hardness =HV 1  =43</th>
<th>Core Hardness =HV 1  =43</th>
<th>Shear Stress Amplitude =τ</th>
<th>Hydrostatic Pressure =σw</th>
<th>Sensitivity to Hydrostatic Pressure =α</th>
<th>Hydrostatic Pressure due to Residual Stresses =k</th>
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<td>Standard</td>
<td>84 wt. %</td>
<td>0.17</td>
<td>685 HV 1</td>
<td>632 HV 1</td>
<td>0.05</td>
<td>0.07</td>
<td>0.09</td>
<td>0.11</td>
</tr>
<tr>
<td>Optimal</td>
<td>91 wt. %</td>
<td>0.19</td>
<td>700 HV 1</td>
<td>652 HV 1</td>
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