# 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 ore 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 thermalchemical heat treatment case hardening [1, 2]. The application of this process leads to high strength materials states such as martensite and compressive residual stresses close to the components surface. The fatigue behaviour of the component is improved. However, function-related construction details have a significant influence on the sub-processes of case hardening. This relates to the carbon diffusion during carburizing and the local heat transfer during quenching [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].





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## 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.



Figure 1: Simulation of case hardening processes, acc. to [6]

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 necessary to create mapping routines to transfer the results between different FE meshes.

The figure 10 shows an overview of the basic procedure for optimizing case hardening processes. The starting point is the identification of all relevant process parameters, such as carburizing and hardening temperature, carbon level and carburizing times. These are subsequently subjected to a sensitivity analysis. 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.



Figure 2: Optimization of case hardening processes

Finally a response-surface optimization of the case hardening process is carried out by using the Metamodel 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 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 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  $p_{RS}$ . A Dang Van equivalent stress is then given by:

$$\sigma_{v,DV} = \tau(t) + \alpha_{DV} \cdot (p(t) + p_{RS})$$
(1)

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

$$f = \max[\eta] = \max\left[\frac{\sigma_{v,DV}}{\tau_W}\right]_{Component} \to MIN$$
(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

С	Mn	Cr	Ni	Мо	Si	s	Р
0.17	0.58	1.56	1.43	0,26	0.24	0.031	0.006
Table 1 Chamical composition of the acce bardening							

Table 1.	Chemical	composition	of the c	ase hard	ening
steel 180	CrNiMo7-6	in wt.%			

<b>Carburizing:</b> Temperature T <sub>C</sub> = 960 °C						
Carbon po- tential	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 <sub>Q</sub> = 860 °C; Medium Oil, 60 °C						
Tempering: Temperature T <sub>T</sub> = 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.

Due to the geometry of the shaft, a high carbon concentration occurs near the corner of the cross hole, Figure 6. This causes a high retained austenite content and a low tempered hardness in this region, Figure 7 and 8, as well as reduced residual stresses. Thereby, compared to the hardened layer of the cross hole, the local fatigue strength is reduced in the high stressed volume of the shaft. The determined Dang Van degree of utilization of the Standard case hardening process of the shaft with bending load is 1.31.



*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

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).



Advanced Latin Hypercupe 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

$$f = \eta^{(i)} = \frac{\sigma_{v,DV}^{(i)}}{\tau_w^{(i)}} \to MIN$$

#### Constraints

- C1:  $\sum t_{CP1} + t_{CP2} + t_{CP3} \le 6000s$
- C2:  $c_{C}(0,8mm)|_{cross hole} \ge 0,25 \text{ Ma.-%C}$
- C3: max.  $c_{c} \leq 0,70$  Ma.-%C

Optimization method

Nonlinear Programming by Quadratic Lagrangian (NLPQL approach) [18]

Figure 10. Overview sensitivity analysis and optimization of the case hardening process

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.



Figure 11. Most important parameters of the Dang Van degree of utilization



Figure 12. Most important parameters of the Dang Van degree of utilization

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.



Figure 13. Most important parameters of the Dang Van degree of utilization



Figure 14. Optimized carburizing process, carbon concentration in wt.%



Figure 15. Optimized carburizing process, dimensionless volume fraction retained austenite









*Figure 16. Optimized carburizing process, Vickers hardness after tempering* 



Figure 17. Optimized carburizing process, axial residual stresses in MPa

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.

Criterium		Standard case hard- ening pro- cess (SP)	Optimized case hard- ening pro- cess (OP)	Differ- ence
High stressed vol-	max. carbon concentration	0.84 wt.%	0.66 wt.%	- 21 %
	max. retained austenite con- tent	0.35	0.23	- 34 %
	max. hardness	632 HV 1	680 HV 1	+ 8 %
	axial residual stresses	- 199.5 MPa	- 267.8 MPa	+ 34 %
Surf dian	ace hardness, neter d = 30 mm	684 HV 1	685 HV 1	-
CHD, GH = 550 HV, diameter d = 30 mm		1.02 mm	0.74 mm	- 28 %
Core hardness		431 HV 1	436 HV 1	-
max. Dang Van utili- zation rate		1.32	1.23	-9%
max. carbon poten- tial		1.18 % C	1.06 % C	- 11 %
Total process time		al process time 290 min		- 52 %

Table 3. Comparison of the investigated variants

## 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
  - $\sigma_{v,DV}$  Dang Van equivalent stress
  - $\tau$  Shear stress amplitude
  - $\tau_w$  Fatigue limit in fully reversed torsion
- $\alpha_{\scriptscriptstyle DV}$  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





### Figure 2:

- $c_c$  Carbon concentration
- $c_{c,0}$  Bulk carbon concentration
- T Temperature
- $T_s$  Transformation start temperature
- $D_c$  Carbon diffusion coefficient
- TTT Isothermal transformation diagram
- V Volume fraction
- $\sigma_{\rm Y}$  Yield strength
- k Phase
- λ Thermal conductivity
- ho Density
- $c_p$  Specific heat
- $\dot{H}$  Strain hardening constant
- $\alpha$  Thermal expansion coefficient
- $\alpha$  Heat transfer coefficient

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