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# Computer simulation of working stress of heat treated steel specimen

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**Analysis and modelling**

## ABSTRACT

**Purpose:** In this paper, the prediction of working stress of quenched and tempered steel has been done. The working stress was characterized by yield strength and fracture toughness. The method of computer simulation of working stress was applied in workpiece of complex form.
**Design/methodology/approach:** Hardness distribution of quenched and tempered workpiece of complex form was predicted by computer simulation of steel quenching using a finite volume method. The algorithm of estimation of yield strength and fracture toughness was based on steel hardness, HV. Yield strength and fracture toughness distributions have been predicted using the Hahn-Rosenfield approach.
**Findings:** It can be concluded that working stress of quenched and tempered steel can be successfully predicted by proposed method. The further experimental investigations are needed for final verification of established model.
**Research limitations/implications:** For efficient estimation of fracture toughness from hardness, additional data about microstructure are needed.
**Practical implications:** Estimation of hardness distribution can be based on time, relevant for structure transformation, i.e., time of cooling from 800 to 500 ºC ($t_{8/5}$). The prediction of distribution of microstructure composition, yield strength, and fracture toughness, can be based on steel hardness.
**Originality/value:** Hardness distribution is predicted by involving the results of simple experimental test, i.e., Jominy-test in numerical modelling of steel quenching.
**Keywords:** Heat treatment; Computer simulation; Microstructure; Yield strength; Fracture toughness

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## 1. Introduction

Main problem in simulation of steel quenching is to establish the efficient way of estimation of physical and mechanical steel properties which have to be involved into the steel quenching model. The numerical simulation of hardness distribution in quenched steel specimen is one of the highest priorities in simulation of phenomena of steel quenching and in prediction of mechanical properties of quenched steel specimen [1-4]. Strength, toughness and fatigue properties could be estimated based on steel hardness [5]. Prediction of hardness, strength, toughness and fatigue properties distribution in quenched steel specimen has been done by computer simulation.

Strength, toughness and fatigue properties of quenched and tempered steel directly depend on steel microstructure. For that reason, two main problems have to be solved in simulation of steel quenching: prediction of temperature field change, and prediction of microstructure composition and mechanical properties.

## 2. Prediction of hardness distribution

Mathematical model of steel quenching can be based on calculated characteristic time of cooling $t_{8/5}$ [6, 7]. The hardness at specimen points can be estimated by the conversion of cooling time results to hardness by using both, the relation between cooling time and distance from the quenched end of *Jominy* specimen and the *Jominy* hardenability curve. The time of cooling at specimen point can be predicted by numerical simulation of cooling using the finite volume method [8, 9].

The referent hardness at specimen points in the quenched and tempered state can be estimated from the referent as-quenched hardness, $HRC_{\mathrm{quenched}}$, by [10-12]:

$$HRC_{tempered} = \frac{HRC_{quenched}}{K} \tag{1}$$

where $K$ is the factor between as-quenched and tempered hardness. Factor $K$ can be expressed by:

$$K = C_1 \cdot t^{n_1} \exp\left[A\left(\frac{a}{T_{temp}}\right)^{n_2} - B\right] \tag{2}$$

where $T_{\mathrm{temp}}$ [K] is the tempering temperature, $t$ [h] is the time of tempering, while $A$, $B$, $C_1$, $a$, $n_1$ and $n_2$ are the material constants.

## 3. Prediction of microstructure distribution

Microstructure composition of steel depends on actual steel hardness that is generally equal:

$$HV = \left\{ \begin{matrix} (\%\,ferrite + \%\,pearlite)HV_{(F+P)} + \\ +(\%bainite)HV_{(B)} + (\%martensite)HV_{(M)} \end{matrix} \right\} \Big/ 100 \tag{3}$$

Amount of phase's portions is equal unity:

$$\{(\%\,ferrite + \%\,pearlite) + \%bainite + \%martensite\}/100 = 1 \tag{4}$$

If the total hardness and hardness of microstructure constituents separately are known, and if the phase fraction of one of microstructure constituents is known, it is not difficult to predict fractions of other phases by the Eq. 3 and Eq. 4. Results of austenite decomposition depend on the chemical composition of steel, severity of cooling, austenitizing temperature and steel history. The austenite decomposition results can be estimated based on time, relevant for structure transformation. The characteristic cooling time, relevant for structure transformation for most structural steels, is the time $t_{8/5}$.

If other heat treatment parameters are constant, the austenite decomposition results in some location of a cooled specimen will depend only on the time $t_{8/5}$. It could be written for *Jominy* specimen that phase hardness depends on chemical composition and cooling rate parameter that corresponds to actual distance $d$ of *Jominy* specimen quenched end. It was adopted that cooling rate parameter is equal to $\log(t_{8/5})$ [13].

$$HV_d^M = HV_{\max}^M - K_M \log \frac{t_{8/5d}^M}{t_{8/5\max}^M} \tag{5}$$

$$HV_d^B = HV_{\max}^B - K_B \log \frac{t_{8/5d}^B}{t_{8/5\max}^B} \tag{6}$$

$$HV_d^{P+F} = HV_N^{P+F} + K_{P+F} \log \frac{t_{8/5N}^{P+F}}{t_{8/5d}^{P+F}} \tag{7}$$

where $N$ is normalizing, and $HV_{\max}^B$ is hardness of lower bainite. Characteristic value of $HV$, $K$ and $t_{8/5}$ in Eq. 5, Eq. 6 and Eq. 7 has to be evaluated for investigated steel combined with *Jominy* test results. Hardness of quenched structures with characteristic percentage of martensite can be predicted by using the diagram of hardness at different percentages of martensite vs. carbon content after Hodge and Orehoski [14] and *Jominy* curve. Similar as for martensite, the regression relations between the time $t_{8/5}$ and characteristic pearlite fractions have to be established [13].

## 4. Prediction of mechanical properties distribution

Mechanical properties of quenched steel or quenched and tempered steel directly depends on degree of quenched steel hardening [5, 12]. Relation between hardness, $HV$, and ultimate tensile stress, $R_{\mathrm{m}}$ [Nmm$^{-2}$] is equal:

$$R_m = 3.3HV \tag{8}$$

Yield strength, $R_{\mathrm{p0.2}}$ [Nmm$^{-2}$], and reduction of area, $Z$ [%], could be estimated from the ultimate tensile stress or hardness [15]:

$$R_e = R_{p0,2} = (0.8 + 0.1C)R_m + 170C\text{-}200 \tag{9}$$

$$Z = 96 - (0.062 - 0.029C)R_m \tag{10}$$

where $C$ is a ratio between the actual hardness and martensite hardness in HRC.

Fracture toughness, $K_{\mathrm{Ic}}$ [MPam$^{1/2}$], can be estimated from the mechanical properties obtained by tensile test. The Hahn-Rosenfield correlation can be successfully used for that purpose [14]:

$$K_{Ic} = \sqrt{\frac{\varepsilon_f n^2 E R_e}{60}} \tag{11}$$

$\varepsilon_{\mathrm{f}}$ is the true fracture strain, $n$ is the strain-hardening exponent, $E$ [Nmm$^{-2}$] is the modulus of elasticity. True fracture strain can be expressed by reduction of area, $Z$:

$$\varepsilon_f = \ln\left(1 - \frac{Z}{100}\right)^{-1} \tag{12}$$

The strain-hardening exponent can be defined by:

$$\frac{R_m}{R_e} - \left(\frac{n}{0.002e}\right)^n \approx 0 \tag{13}$$

Fatigue resistance properties could be estimated based on yield strength and microstructural constitution. The effect of tempering and microstructure composition is relatively small for region 2 growth rates, but the effect may be large near the threshold in region 1 growth rates. Continuous ferrite phase reduces fatigue crack growth resistance near the threshold. So, substantial reducing in fatigue crack growth resistance near the threshold is possible with formation of continuous network of ferrite phase.

Grain size is another way of fatigue threshold control. Large grain size has the beneficial effect on thresholds for low-strength steels but the negligible effect for high-strength steels. Controlling microstructural unit for low- to medium-strength steels is reversed plastic zone size, $R_{p\pm}$, which is useful to compare with the grain size. Using the twice the plane-strain plastic radius and twice the yield stress, due to the stress reversal gives [16]:

$$R_{p\pm} = \frac{2\Delta K^2}{6\pi(2R_e)^2} \tag{14}$$

Cyclic slip will not proceed if the grain size, $d$, is greater than the reversed plastic zone size. Substituting that $d = R_{p\pm}$, the fatigue crack initiation threshold, $\Delta K_{th}$, below which fatigue cracks would not initiate at specimen points in the quenched and tempered state, can be estimated by:

$$K_{th} = R_e(12\pi d)^{1/2} \tag{15}$$

Including the microstructure effects, it could be find out that:

$$\Delta K_{th} = nAR_e d^{1/2} \tag{16}$$

where $n$ is the parameter depending of ferrite volume, while $A$ is the material constant.

## 5. Application

The established method is applied in failure analysis of quenched and tempered steel shaft made of steel 42CrMo4 (DIN). The chemical composition of investigated steel is shown in Table 1. *Jominy* test results of steel 42CrMo4 are shown in Table 2.

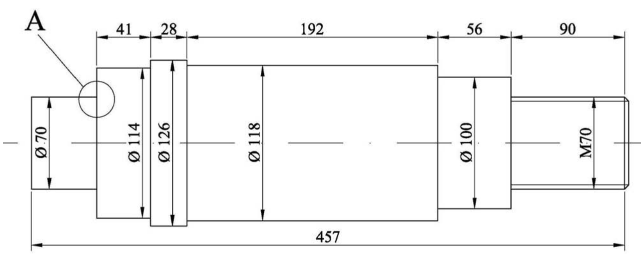


Fig. 1. Workpiece geometry

Table 1.
Chemical composition of steel 42CrMo4 (DIN)

| Chemical composition [wt.%] | | | | | | |
|---|---|---|---|---|---|---|
| C | Si | Mn | P | S | Cr | Mo |
| 0.38 | 0.23 | 0.64 | 0.019 | 0.013 | 0.99 | 0.16 |

Table 2.
*Jominy* test results of steel 42CrMo4

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Jominy* distance, mm | 1.5 | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 20 | 25 | 30 |
| Hardness HV | 610 | 605 | 590 | 576 | 555 | 524 | 487 | 446 | 379 | 344 | 324 |
| *Jominy* distance, mm | 35 | 40 | 45 | 50 | 55 | 60 | 65 | 70 | 75 | 80 | - |
| Hardness HV | 311 | 303 | 297 | 293 | 292 | 291 | 289 | 288 | 288 | 288 | - |

Table 3.
Parameters of heat treatment of broken shaft

| Quenching | | | Tempering | | |
|---|---|---|---|---|---|
| Temperature | Time | Media | Temperature | Time | Media |
| 850 °C | 1 hour | oil, H=0.25 | 600 °C | 1 hour | air |

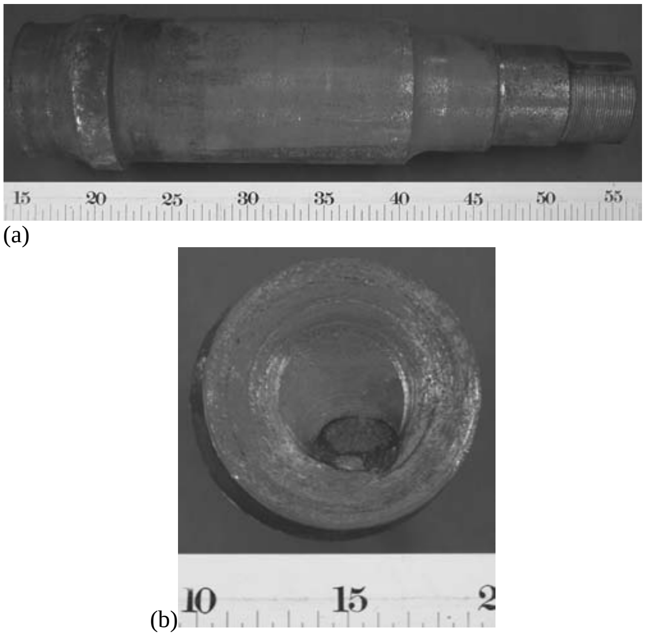


Fig. 2. Photographs of broken shaft

Photographs of broken shaft and of its failure surface are shown in Fig. 2a and Fig. 2b, respectively.

The broken shaft was treated by heat treatment in which, after heating to 850 °C and holding for 1 hour, the shaft was quenched in oil with the severity of quenching $H$ = 0.25. The tempering temperature was 600 °C. Parameters of heat treatment of broken shaft are shown in Table 3.

The shaft treated by the proposed heat treatment was broken after short time of application.

It is visible that failure started in critical location A (Fig. 1) and propagated by cycle fatigue with very low stress intensity.

Based on proposed mathematical model, computer simulation of microstructure composition and fatigue resistance was made.

Calculated microstructure compositions vs. time $t_{8/5}$ of investigated steel is shown in Fig. 3.

Distributions of microstructure and mechanical properties fields of treated shaft (Table 3) are shown in Fig. 4.

Heat transfer coefficients and heat conductivity coefficient as well as heat capacity of quenched steel were calculated by the special method of calibration [6, 7].

The predicted values of as-quenched microstructure and mechanical properties of the workpiece are given in Table 4 for quenching in oil with the severity of quenching $H = 0.25$.

Very heterogeneous as-quenched microstructure in surface locations is achieved by quenching in oil with the severity of quenching $H = 0.25$ (Fig. 4), which leads to reduced fatigue crack initiation threshold.

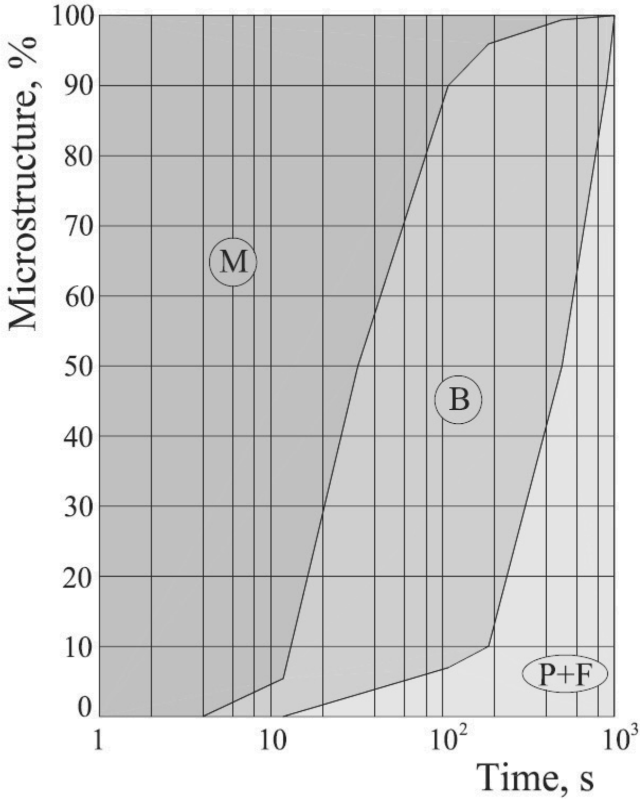


Fig. 3. Microstructure compositions vs. time $t_{8/5}$; (P+F) - Pearlite + Ferrite; B - Bainite; M – Martensite

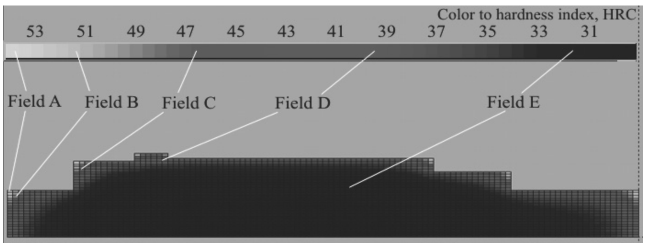


Fig. 4. Distributions of microstructure and mechanical properties fields of the workpiece for quenching in oil; $H = 0.25$

Table 4.
Microstructure and mechanical properties of the workpiece for quenching in oil; $H = 0.25$

| Properties | | Field in Figure 4 | | | | |
|---|---|---|---|---|---|---|
| | | A | B | C | D | E |
| Hardness [HV] | | 610-575 | 575-510 | 510-440 | 440-340 | 340-290 |
| Yield strength $R_e$ [Nmm$^{-2}$] | | 2013-1898 | 1898-1683 | 1683-1452 | 1452-1122 | 1122-957 |
| Fracture toughness $K_{Ic}$ [MPam$^{1/2}$] | | 64-68 | 68-77 | 77-88 | 88-106 | 106-118 |
| Phase fractions [%] | F+P | 0 | 0 | 0 | 0 | 0-12 |
| | B | 1-2 | 2-19 | 19-42 | 42-74 | 74-83 |
| | M | 99-98 | 98-81 | 81-58 | 58-26 | 26-5 |

Table 5.
Parameters of heat treatment of shaft to obtain higher fatigue limit

| Quenching | | | Tempering | | |
|---|---|---|---|---|---|
| Temperature | Time | Media | Temperature | Time | Media |
| 850 °C | 1 hour | oil, H = 0.7 | 600 °C | 1 hour | air |

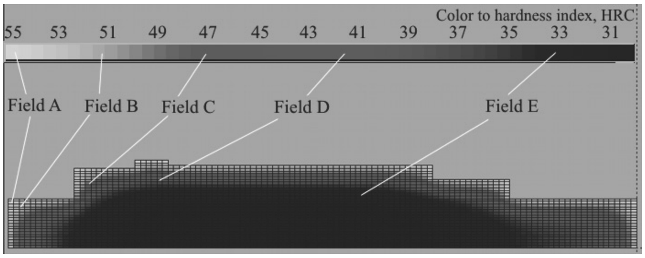


Fig. 5. Distributions of microstructure and mechanical properties fields of the workpiece for quenching in oil; $H = 0.7$

More homogeneous as-quenched microstructure in surface location could be achieve by quenching in oil with higher severity of quenching for example of $H = 0.7$.

In propose to made shaft with the higher fatigue limit, shaft was treated with the same heat treatment but was quenched in oil with severity of quenching $H = 0.7$. Parameters of this heat treatment are shown in Table 5.

Table 6.
Microstructure and mechanical properties of the workpiece for quenching in oil; $H = 0.7$

| Properties | | Field in Figure 5 | | | | |
|---|---|---|---|---|---|---|
| | | A | B | C | D | E |
| Hardness [HV] | | 610-575 | 575-510 | 510-453 | 453-370 | 370-298 |
| Yield strength $R_e$ [Nmm$^{-2}$] | | 2013-1898 | 1898-1683 | 1683-1495 | 1495-1221 | 1221-983 |
| Fracture toughness $K_{Ic}$ [MPam$^{1/2}$] | | 64-68 | 68-77 | 77-86 | 88-100 | 100-116 |
| Phase fractions [%] | F+P | 0 | 0 | 0 | 0 | 0-10 |
| | B | 1-2 | 2-19 | 19-37 | 37-64 | 64-81 |
| | M | 99-98 | 98-81 | 81-63 | 63-36 | 36-9 |

Distributions of microstructure and mechanical properties fields of treated shaft (Table 5) are shown in Fig. 5.

The predicted values of as-quenched microstructure and mechanical properties of the workpiece for quenching in oil with the severity of quenching $H = 0.7$ are given in Table 6.
The predicted values of mechanical properties of the workpiece quenched in oil with severity of quenching $H = 0.7$, subsequently tempered at 600 °C, are given in Table 7.

Table 7.
Mechanical properties of the quenched ($H = 0.7$) and tempered workpiece

| Properties | Field in Figure 5 | | | | |
|---|---|---|---|---|---|
| | A | B | C | D | E |
| Hardness [HV] | 291-290 | 290-280 | 280-272 | 272-256 | 256-234 |
| Yield strength $R_e$ [$Nmm^{-2}$] | 960-957 | 957-924 | 924-898 | 898-845 | 845-772 |
| Fracture toughness $K_{Ic}$ [$MPam^{1/2}$] | 117-118 | 118-120 | 120-122 | 122-126 | 126-132 |
| Fatigue threshold $\Delta K_{th}$ [$MPam^{1/2}$] | 22.6-22.5 | 22.5-21.8 | 21.8-21.2 | 21.2-20.1 | 20.1-10.5 |

It is visible that in locations near the workpiece surface the as-quenched microstructure of homogeneous martensite is achieved by quenching in oil with severity of quenching $H = 0.7$ (Fig. 5).

By economical aspects of simulation of investigated shaft manufacturing, most suitable shaft manufacture process is to manufacture the shaft from the quenched and tempered bar of 130 mm diameter. But in this case, in critical location A (Fig. 1), heterogeneous microstructure of ferrite, perlite, bainite and martensite will be received, with very low fatigue limit.

## 6. Conclusions

A developed mathematical model has been applied in failure analysis of a quenched and tempered steel shaft. The model is based on finite volume method. The hardness distribution in the quenched workpiece is estimated based on time of cooling from 800 to 500 °C, $t_{8/5}$, and on results of the *Jominy* test. The prediction of distribution of microstructure composition, yield strength, and fracture toughness is based on steel hardness. Fatigue resistance properties are based on yield strength and microstructural constitution.

Using a numerical simulation of microstructure and mechanical properties, it was established that better results of quenching can be achieved by quenching in oil with higher severity of quenching.

It can be concluded that mechanical properties of quenched and tempered steel workpieces can be successfully calculated by the proposed method, and that proposed method can be successfully applied in failure analysis of quenched and tempered steel workpieces. For efficient estimation of fracture toughness and fatigue resistance additional data about microstructure are needed.

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