18th IFHTSE CONGRESS
International Federation for Heat Treatment and Surface Engineering
IFHTSE

ANAIS
PROCEEDINGS
ISSN 1516-392X

MATHEMATICAL MODELLING AND COMPUTER SIMULATION OF FATIGUE PROPERTIES OF QUENCHED AND TEMPERED STEEL[1]

Božo Smoljan[2]
Dario Iljkić[2]
Furio Traven[2]
Josipa Mrša[3]

Abstract

The engineering and economical aspects of optimization of steel shaft quenching and tempering were investigated. The mathematical model and method of computer simulation for prediction of fatigue properties quenched and tempered steel has been developed. Computer simulation of fatigue properties quenched and tempered steel has been applied in optimization of quenching and tempering of steel shaft. Proper heat treatment process was accepted based on economical analyse. Fatigue properties of quenched and tempered steel have been predicted based on microstructure composition and yield strength. Microstructure composition and yield strength have been predicted based on as-quenched hardness. Distribution of as-quenched hardness in workpiece was predicted by computer simulation of steel quenching using a finite volume method. The as-quenched hardness is estimated based on time of cooling and on Jominy test results. It was taken into account that mechanical properties of quenched steel directly depend on hardness and degree of hardening and microstructural constituents. Using a numerical simulation of microstructure and mechanical properties, it was found out that best fatigue properties investigated shaft has if it was machined or formed on proper geometry before proper quenching and tempering. By economical analise of investigated shaft manufacturing was found out that most suitable shaft manufacture process is to manufacture the shaft from the quenched and tempered bar. But in this case, heterogeneous microstruture of ferrite, perlite, bainite and martensite, with very low fatigue limit could appeare at some critical locations.

Key words: Quenching; Tempering; Computer simulation; Fatigue limit.

[1] *Technical contribution to the 18th IFHTSE Congress - International Federation for Heat Treatment and Surface Engineering, 2010 July 26-30th, Rio de Janeiro, RJ, Brazil.*

[2] *University of Rijeka, Faculty of Engineering, Department of Materials Science and Engineering, Vukovarska 58, 51000 Rijeka, Croatia.*

[3] *University of Rijeka, Faculty of Economics, Ivana Filipovića 4, 51000 Rijeka, Croatia.*

1 INTRODUCTION

The numerical simulation of hardness distribution in quenched steel specimen has one of the highest priorities in simulation of phenomena of steel quenching, and in prediction of mechanical properties of quenched steel specimen. Hardness, yield strength, toughness and fatigue properties are in relation with each other.[1] Hardness distribution in quenched steel specimen could be predicted by computer simulation, and after that yield strength, toughness and fatigue properties can be predicted based on hardness distribution.

Fatigue properties of quenched and tempered steel mostly depend on steel microstructure. For that reason, there are two main tasks that should be solved in simulation of steel quenching: (a) prediction of temperature field change; (b) prediction of microstructure composition. Mathematical model of microstructure composition in quenched steel can be based on characteristic time of cooling from 800 to 500°C ($t_{8/5}$) during the quenching.[2,3,4] 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.[4,5,6]

2 PREDICTION OF QUENCHED AND TEMPERED STEEL HARDNESS

The referent hardness at specimen points in the quenched and tempered state can be estimated from the referent as-quenched hardness, HRC_{quenched}, by:[7,8]

$$HRC_{tempered} = \frac{HRC_{quenched}}{K} \qquad (1)$$

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

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

where T_{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. Referent quenched and tempered hardness depends on minimum Rockwell C hardness which could be achieved in actual steel. Minimum Rockwell C hardness for actual steel is depends on chemical composition and tempering temperature.

3 PREDICTION OF QUENCHED AND TEMPERED STEEL MICROSTRUCTURE

Microstructure composition of as-quenched steel depends on the chemical composition, severity of cooling, austenitizing temperature and steel history. Actual steel hardness depends on microstructure composition:

$$HV = \{(\% ferrite + \% pearlite)HV_{(F+P)} + (\% bainite)HV_{(B)} + (\% martensite)HV_{(M)}\}/100 \quad (3)$$

Amount of phase's portions is equal unity:

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

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 at some locations 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 $\log(t_{8/5})$.[9]

$$HV_d^M = HV_{\max}^M - K_M \log\frac{t_{8/5d}^M}{t_{8/5\max}^M}, \quad (5)$$

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

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

where *N* is normalizing, and $HV_{\max}^B$ is hardness of lower bainite. Characteristic value of *HV*, K_M, K_B, K_{P+F} 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[10] and *Jominy* curve. Similar as for martensite, the regression relations between the time $t_{8/5}$ and characteristic pearlite fractions have to be established.[9] 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).

4 PREDICTION OF QUENCHED AND TEMPERED STEEL FATIGUE PROPERTIES

Relation between hardness, *HV*, and yield strength, $R_{p0.2}$/MPa is equal to:[11]

$$R_e = R_{p0,2} = (0.24 + 0.03C)HV + 170C\text{-}200 \quad (8)$$

Coefficient *C* which is ratio between the actual hardness and hardness of martensite in Rockwell C hardness, should be taken in account since as-quenched and quenched and tempered steel properties depends on degree of quenched steel hardening.[1]

In comparison with yield strength the fatigue resistance properties additionally depend on microstructure, especially it depend on ferrite phase composition. 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. With segregation of ferrite phase in form of continuous network substantial reducing in fatigue crack growth resistance near the threshold is possible.

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. 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, ΔK_{th}, below which fatigue cracks would not initiate at specimen points in the quenched and tempered state, can be estimated by:[12]

$$\Delta K_{th} = R_e (12\pi d)^{1/2} \quad (9)$$

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

$$\Delta K_{th} = nAR_e d^{1/2} \quad (10)$$

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

5 APPLICATION

The established method for prediction of fatigue resistance of quenched and tempered steel is applied in design of heat treatment of steel shaft made of steel 42CrMo4 (DIN). The chemical composition of steel is 0.38 %C, 0.23 %Si, 0.64 %Mn, 0.019 %P, 0.013 %S, 0.99 %Cr and 0.16 %Mo. *Jominy* test results of steel 42CrMo4 are shown in Table 1.

Table 1. *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	-

Based on the *Jominy* test results the diagram of microstructure composition in dependency of cooling times from 800 to 500°C, $t_{8/5}$, was done. Calculated microstructure compositions vs. time $t_{8/5}$ of investigated steel are shown in Figure 1.

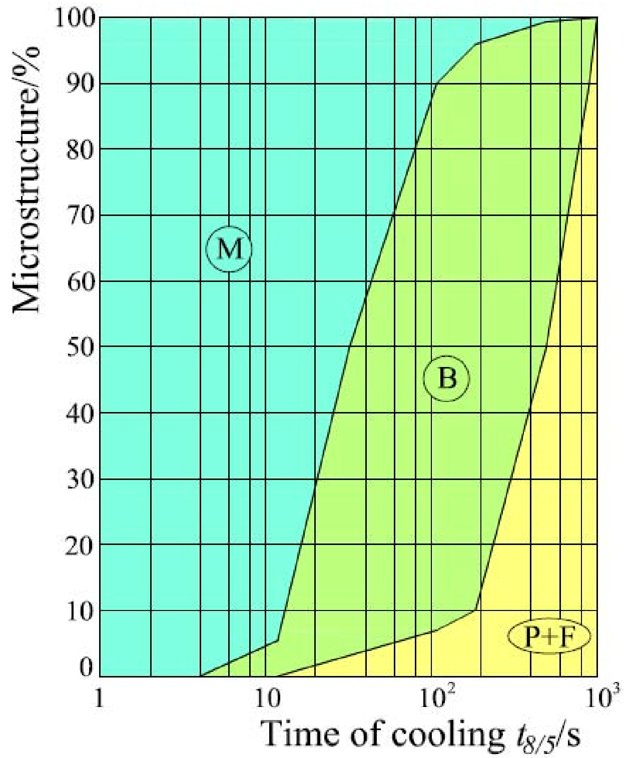


Figure 1. Microstructure compositions vs. time $t_{8/5}$; (P+F) - Pearlite + Ferrite; B - Bainite; M – Martensite.

Geometry of steel shaft is shown in Figure 2a. Three different manufacture processes of the steel shaft were designed. In the first manufacture process before final cutting process the shaft was quenched in oil with the severity of quenching equal to 0.25. In the second manufacture process the shaft was quenched in oil with the severity of quenching equal to 0.4. And finally in the third process steel shaft was manufacture from the quenched and tempered bar of diameter of 130 mm. The steel shaft in the third process was quenched in oil with the severity of quenching equal to 0.4. The tempering temperature in all three processes was 600°C. Geometry of steel shaft prepared for the heat treating processes are shown in Figure 2b and Figure 2c. In Figure 2b and Figure 2c geometry of steel shaft after final machining is shown by dashed line. Parameters of heat treatment processes are shown in Table 2.

Table 2. Parameters of heat treating processes of steel shaft

Process	Machining	Quenching		Tempering	
		Temperature	Quenchant	Temperature	Time
1	yes	850°C	oil – no agitation H = 0.25	600°C	1 hour
2	yes	850°C	oil – good agitation H = 0.4	600°C	1 hour
3	no	850°C	oil – good agitation H = 0.4	600°C	1 hour

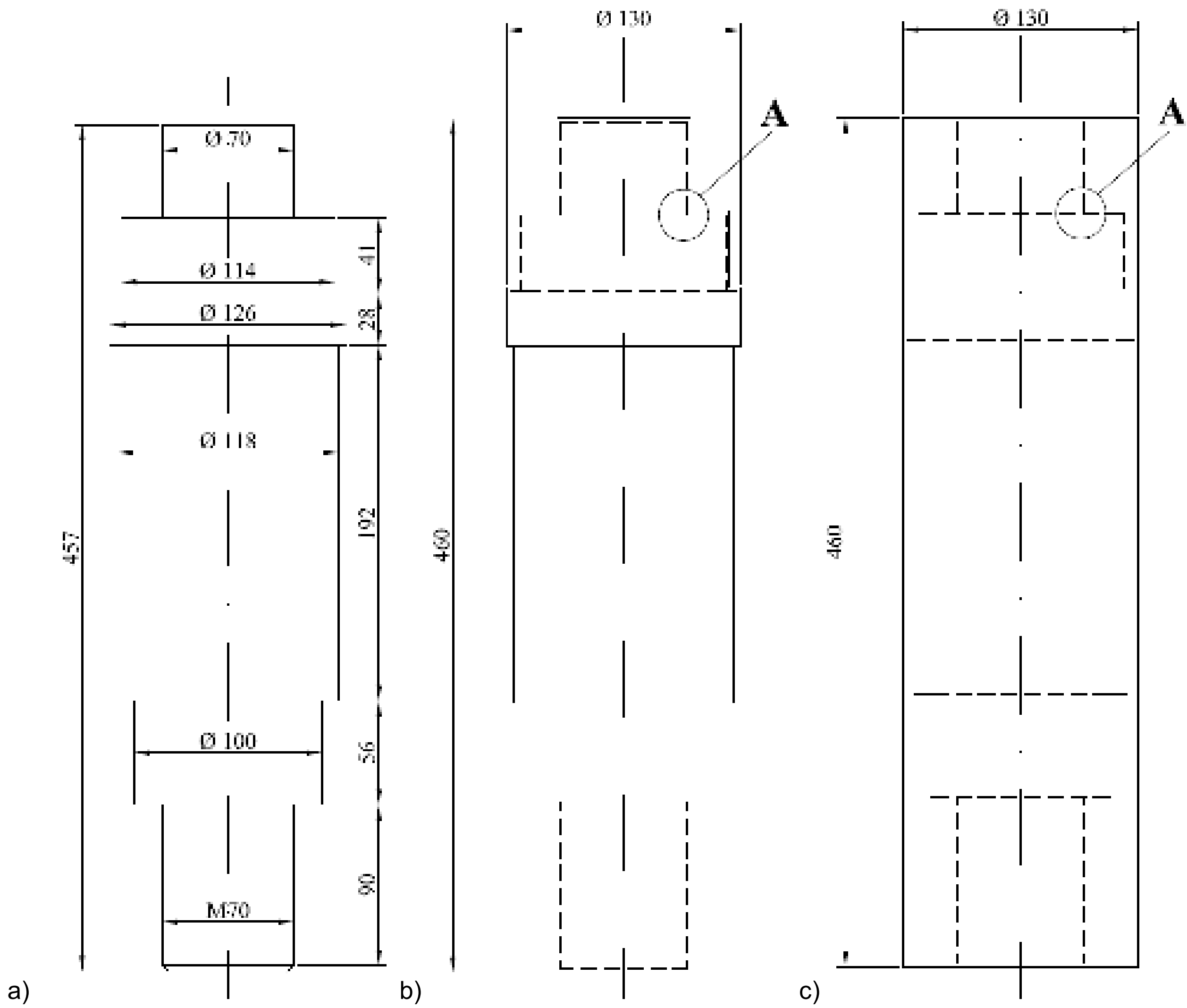


Figure 2. a) geometry of steel shaft, b) geometry of steel shaft prepared for processes 1 and 2, c) geometry of steel shaft prepared for process 3.

Distributions of hardness of as-quenched workpieces with different shapes are shown in Figure 3. Distributions of hardness and yield strength of quenched and tempered workpieces treated by process 1, 2 and 3, respectively, are shown in Figure 4, Figure 5 and Figure 6.

ANAIS
PROCEEDINGS
ISSN 1516-392X

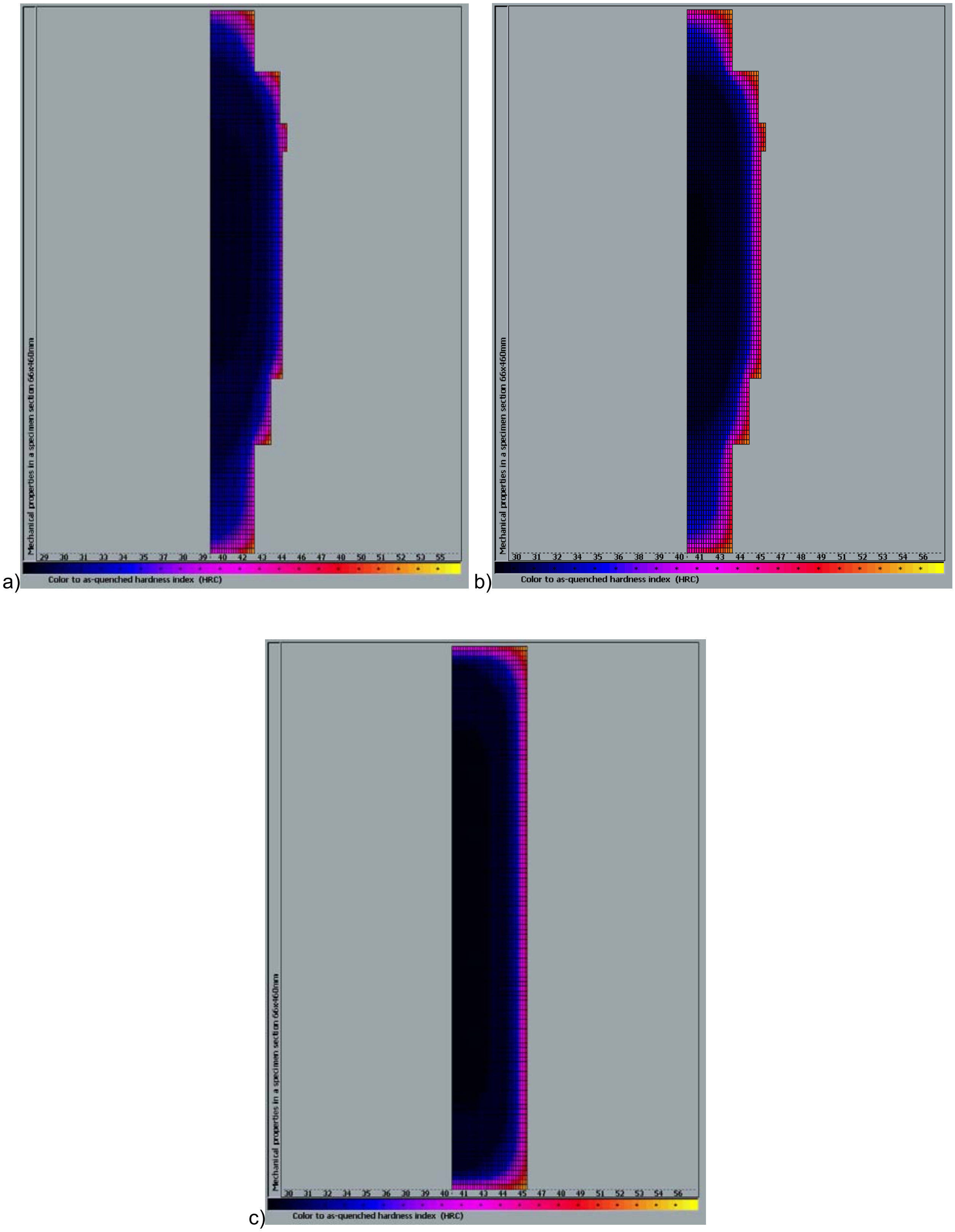
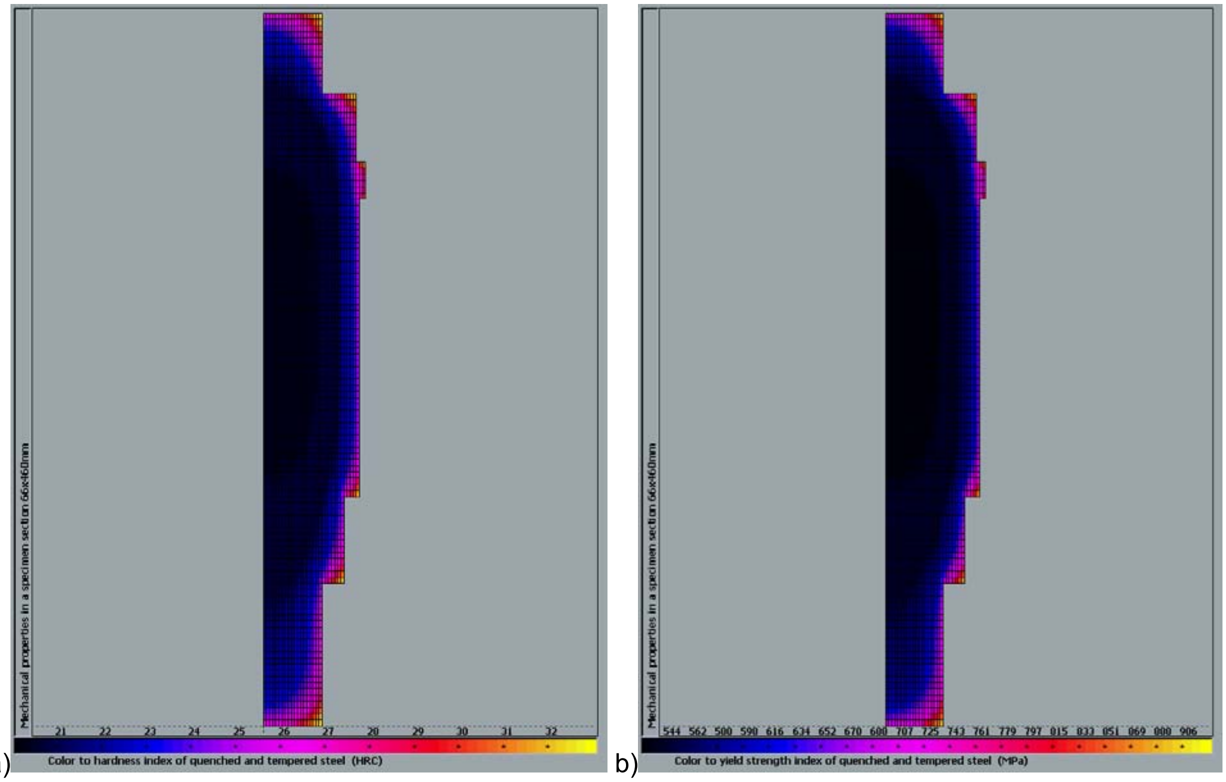


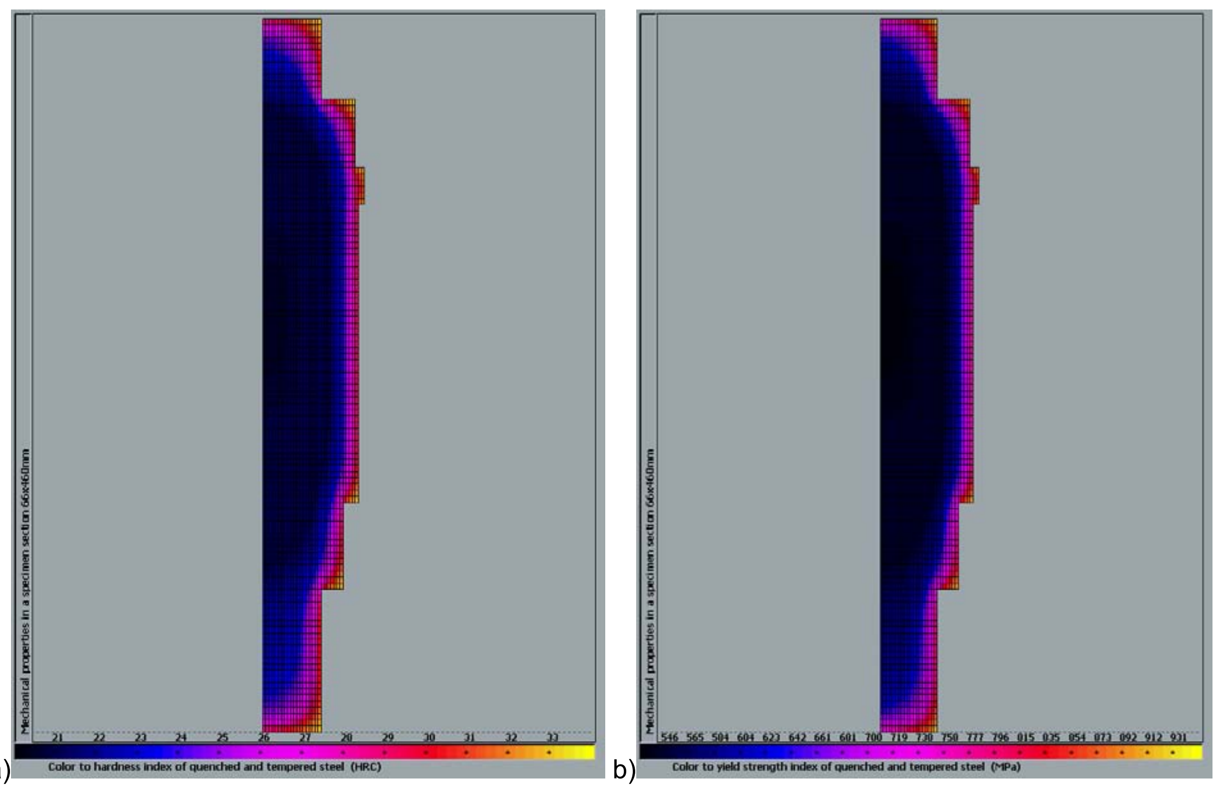
Figure 3. Distributions of hardness of as-quenched workpieces, a) process 1, b) process 2, c) process 3.

ISSN 1516-392X



a) b)

Figure 4. Distributions of mechanical properties of quenched and tempered workpiece treated by process 1, a) hardness, b) yield strength.



a) b)

Figure 5. Distributions of mechanical properties of quenched and tempered workpiece treated by process 2, a) hardness, b) yield strength.

ISSN 1516-392X

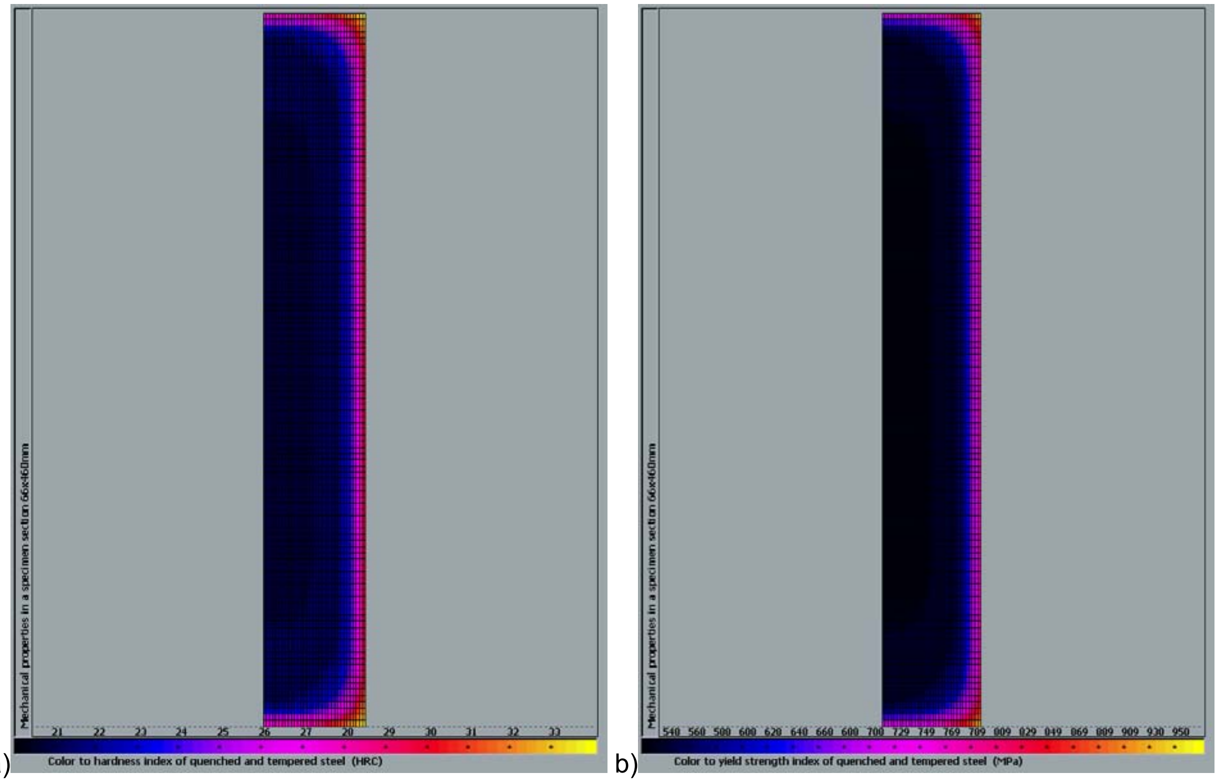


Figure 6. Distributions of mechanical properties of quenched and tempered workpiece treated by process 3, a) hardness, b) yield strength.

Location A is a critical place for possible fatigue crack growth (Figure 2b and Figure 2c). Predicted microstructure composition and fatigue resistance properties at location A are shown in Table 3.

Table 3. Microstructure composition and fatigue resistance properties for location A

Properties		Process (Table 2)		
		1	2	3
Hardness/HRC		41	48	30
Yield strength R_e/MPa		696	794	541
Phase fractions/%	F+P	3.7	2.1	9.2
	B	52	33.3	85.1
	M	44.3	64.6	5.7
Fatigue threshold, ΔK_{th}/MPam$^{1/2}$		13.7	16.7	9.2

It is visible that at location A the as-quenched microstructure of homogeneous martensite and bainite can be achieved only by process 2 or by process where workpiece was machined before quenching in oil with the severity of quenching equal to 0.4 (Figure 3b). More heterogeneous as-quenched microstructure at surface locations will be achieved by processes 1 and 3, which leads to reduced fatigue crack initiation threshold.

By economical aspects of simulation of investigated shaft manufacturing, most suitable shaft manufacture process is process 3, which means to manufacture the shaft from the quenched and tempered bar of diameter of 130 mm. But in this case, at critical location A (Figure 2b and Figure 2c), heterogeneous microstructure of ferrite, perlite, bainite and martensite will be received, with lowest fatigue limit. Taking in account all circumstances it could be found out that proper process for manufacturing of the investigated shaft should be process 2.

6 CONCLUSIONS

A mathematical model for prediction of fatigue resistance of quenched and tempered steel was developed. The model is based on finite volume method. The mathematical model has been applied in optimization of the manufacturing of a quenched and tempered steel shaft. 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 and yield strength is based on steel hardness. Fatigue resistance properties are predicted based on yield strength and microstructural constitution.

It can be concluded that mechanical properties of quenched and tempered steel workpieces can be successfully calculated by the proposed method. For more efficient estimation of fatigue resistance, additional data about microstructure are needed. Proposed method can be successfully applied in optimization of the manufacturing of a quenched and tempered steel shaft.

Using a numerical simulation of microstructure and mechanical properties, it was established that proper manufacture process of investigated shaft manufacturing should consists of machining or forming in proper geometry followed by proper quenching and tempering. For good fatigue resistance steel shaft should be quenched in oil with good agitation.

REFERENCES

1 SMOLJAN, B. Prediction of mechanical properties and microstructure distribution of quenched and tempered steel shaft. *Journal of Materials Processing Technology*, v. 175, no. 1, p. 393-397, 2006.

2 SMOLJAN, B. The calibration of the heat conductivity coefficient in mathematical model of steel quenching. *Proceedings of MicroCAD`99*, Miskolc, February 24.-25., 1999.

3 SMOLJAN, B. The calibration of the mathematical model of steel quenching. *Proceedings of 5th World Seminar on Heat Treatment and Surface Engineering*, Isfahan, September 13.-16., 1995.

4 SMOLJAN, B., ILJKIĆ, D., SMOKVINA HANZA, S. Computer simulation of working stress of heat treated steel specimen. *Journal of Achievements in Materials and Manufacturing Engineering*, vol. 34, no. 2, p. 152-158, 2009.

5 PATANKAR, S. *Numerical Heat Transfer and Fluid Flow*, New York: McGraw Hill Book Company, p. 60, ISBN 0-07-048740-5, 1980.

6 SMOLJAN, B. Numerical simulation of as-quenched hardness in a steel specimen of complex form. *Communications in Numerical Methods in Engineering*, v. 14, no. 1, p. 277-285, 1998.

7 SMOLJAN, B., SMOKVINA HANZA, S., ILJKIĆ, D., TOTTEN, G. E., FELDE, I. Computer simulation of mechanical properties of steel dies. *Proceedings of 2nd International Conference on Heat Treatment and Surface Engineering of Tools and Dies*, Bled, May 25.-28., 2008.

8 RETI, T., FELDE, I., GUERRERO, M., SARMIENTO, S. Using generalized time-temperature parameters for predicting the hardness change occurring during tempering. *Proceedings of the International Conference on New Challenges in Heat Treatment and Surface Engineering (Conference in honour of Prof. Božidar Liščić)*, Dubrovnik-Cavtat, June 8.-12., 2009.

9 SMOLJAN, B. Computer simulation of microstructure transformation during the quenching. *Proceedings of 1st International Surface Engineering Congress and 13th IFHTSE Congress (ASM International)*, Ohio, September 7.-10., 2002.

10 SMOLJAN, B., BUTKOVIĆ, M. Simulation of mechanical properties of hardened steel. *Proceedings of MicroCAD '98*, Miskolc, February 25.-28., 1998.

11 SMOLJAN, B. Numerical simulation of steel quenching. *Journal of Materials Engineering and Performance*, v. 11, no. 1, p. 75-80, 2002.

12 WILSON, A. et al. *Fatigue and Fracture Resistance of ferrous Alloys* in ASM Handbook-Volume 19: Fatigue and Fracture, Material Park, OH: ASM International, p. 591, ISBN 0-87170-385-8, 1996.