Computer simulation of quenched and tempered steel properties

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Received 08.04.2011; published in revised form 01.06.2011

ABSTRACT

Purpose: The algorithm of estimation of mechanical properties based on steel hardness has been established.
Design/methodology/approach: Numerical modelling of hardness distribution in as-quenched steel specimen was performed by involving the results of simple experimental test, i.e., Jominy-test. Hardness of quenched and tempered steel has been expressed as function of maximal hardness of actual steel and hardness of actual steel with 50% of martensite in microstructure, according to the time and temperature of tempering. After that distribution of other relevant mechanical properties was predicted based on predicted as-quenched and tempered hardness of steel. Experimental investigation has been performed on low alloy steel. The established procedure for estimation of quenched and tempered properties of steel has been applied in computer simulation of mechanical properties of quenched and tempered steel workpiece of complex form.
Findings: Algorithm of estimation of hardness of quenched and tempered steel was improved. It can be concluded that working stress of quenched and tempered shaft can be successfully predicted by proposed method. The proposed computer simulation method could be applied in failure prevention.
Research limitations/implications: The research was focused only on carbon and low alloyed heat treatable steels.
Practical implications: The established algorithms can be used for prediction of mechanical properties in heat treating practice. Estimation of as-quenched hardness distribution is based on time, relevant for structure transformation, i.e., time of cooling from 800 to 500°C ($t_{8/5}$). The hardness in the quenched and tempered state is estimated from the as-quenched hardness. The prediction of yield strength and toughness of steel is 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: Quenching; Tempering; Computer simulation; Hardness; Mechanical properties

1. Introduction

It is known that mechanical properties, i.e., hardness, yield strength, toughness and fatigue properties are in relation with each other [1]. 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 [2-5]. Other mechanical properties of steel can be predicted based on hardness distribution. All mechanical properties of quenched steel directly
depend on the degree of quenched steel hardening [6].

Mathematical model of steel quenching results can be based on calculated characteristic time of cooling, \( t_{5/8} \) [7,8]. First, the characteristic time of cooling, \( t_{5/8} \), should be calculated. The time of cooling at specimen point can be predicted by numerical simulation of cooling using the finite volume method [9-10]. After that, the hardness at specimen points can be estimated by the conversion of cooling time, \( t_{5/8} \), 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 hardness of the quenched and tempered steel can be estimated based on as-quenched hardness [6].

Usually two main problems have to be solved in simulation of steel quenching. First, it is simulation of temperature field change, and based on it, second, simulation of mechanical properties should be done.

### 2. Algorithm for prediction of steel hardness

The numerical simulation of quenching results is based on finite volume method [9-10]. The hardness distribution results in the quenched workpiece are estimated based on calculated time of cooling from 800 to 500°C, \( t_{5/8} \), and based experimentally obtained results of the Jominy test. The hardness distribution of quenched steel can be estimated based on kinetic parameters, relevant for microstructure transformation. It is known that usually, if the cooling time, \( t_{5/8} \), in two different steel specimens is equal to each other, the hardness of these two specimens could be equal to each other. The cooling time, \( t_{5/8} \), was predicted by numerical modelling using the finite volume method. Because there is a fixed relation between the cooling time, \( t_{5/8} \), and the distance from the quenched end of the Jominy specimen, for each time, \( t_{5/8} \), the corresponding Jominy distance can be read. By this reason Jominy test results could be applied in simulation of hardness of quenched steel workpiece. In the developed computer simulation of steel quenching, the hardness at different workpiece points is estimated by the conversion of the cooling time, \( t_{5/8} \), to the hardness. Cooling time, \( t_{5/8} \), is calculated in Jominy-specimen and concrete workpiece in question, but hardness is experimentally evaluated by Jominy-test. The next step is to read the hardness at the relevant Jominy distance from the Jominy hardenability curve of the concrete steel in question. The cooling time, \( t_{5/8} \), is converted to hardness using the relation between cooling time, \( t_{5/8} \), and distance from the quenched end of the Jominy specimen [11]. The prediction of distribution of steel mechanical properties is based on steel hardness.

The hardness at specimen points in the quenched and tempered state can be estimated from the as-quenched hardness, \( HRC_{\text{quenched}} \), by [6,12]:

\[
HRC_{\text{tempered}} = \frac{HRC_{\text{quenched}} - HRC_{\text{min}}}{K} + HRC_{\text{min}}
\]

(1)

where: \( HRC_{\text{min}} \) is the materials constant, \( K \) is the factor between as-quenched and tempered hardness.

High hardness decrease at tempering much more than low hardness, the prediction is more precise if the degree of hardening is accounted. Except of degree of hardening, hardness after tempering depends on some other steel properties, as well as, diffusivity properties. Since hardenability properties also depends partially on diffusivity properties, it reasonably to found out relation between some hardenability properties and quenched and tempered hardness. Factor \( K \) can be expressed by [13]:

\[
K = \exp\left[ AB \left( \frac{T_{\text{tempered}}}{t} \right)^m \right]
\]

(2)

where \( T_{\text{tempered}}/K \) is the referent tempering temperature.

The algorithm for prediction of hardness of tempered and quenched steel given by Equation 1 and Equation 2 was established by regression analysis. Equations (1) and (2) are valid for carbon and low alloy steel. For the time of tempering of 1 hour the referent tempering temperature is equal to the tempering temperature. For other time of tempering the referent tempering temperature depends on time of tempering. The material constant, \( A \), depends on degree of hardening and chemical composition. Material constants, \( B, a, \) and \( n \), depend on chemical composition. These material constants are established by regression analysis of hardness of quenched and tempered steel. For investigated steel these material constants are equal to: \( B = 0.3433, a = 808.69 \) and \( n = 6.7484 \) [14].

Results of prediction of hardness of tempered and quenched steel received by established algorithm was compared with results received by algorithm proposed by German standard DIN 17021:

\[
HRC_{\text{quenched}} = \left( T_{\text{tempered}} / 167 - 1.2 \right) HRC_{\text{tempered}} - 17
\]

(3)

and by algorithm established by Just E. [15, 16]:

\[
HRC_{\text{quenched}} = 8 + (HRC_{\text{tempered}} - 8) \exp[C(T_{\text{tempered}}/917)^{d}] 
\]

(4)

Regression analysis made on numerous carbon and low alloyed steels showed that R-square for established algorithm (Equation 1, Equation 2) was equal to 0.9567 (Figure 1). It is much higher than R-square for two other algorithms. For algorithm accepted by German standard DIN 17021 (Equation 3), R-square was equal to 0.7541 (Figure 2a), and for algorithm established by Just E. (Equation 4) R-square was equal to 0.9093 (Figure 2b).

### 3. Algorithm for prediction of steel mechanical properties

One most tested relation in material science is relation between hardness and ultimate tensile stress. Relation between hardness \( HV \) and ultimate tensile stress, \( R_p/Nm^2 \), is equal to:

\[
R_p = 0.3433 \times 10^{0.23 HRC}
\]

\[
R_p = 0.3433 \times 10^{0.23 HRC}
\]
$R_m = 3.3HV$  \hspace{1cm} (5)

By experimental work it was found out that relation given by Equation (8) is valid for tensile strength range between 400-2500 MPa \[17\].

Other mechanical properties of quenched steel or quenched and tempered steel directly depends on ultimate tensile stress, $R_m$/MPa and degree of quenched steel hardening, $C$ \[1,18\]. Yield strength, $R_{0.2}$/Nmm$^2$, percent elongation, $A\%$, and percent reduction of area, $Z\%$, could be estimated from the ultimate tensile stress or hardness \[15\]:

$$R_e = R_{pt,2} = (0.8 + 0.1C)R_m + 170C - 200$$  \hspace{1cm} (6)

$$A = 46 - (0.04 - 0.012C)R_m$$  \hspace{1cm} (7)

$$Z = 96 - (0.062 - 0.029C)R_m$$  \hspace{1cm} (8)

where coefficient $C$ is ratio between the actual hardness and hardness of martensite in Rockwell C hardness.

Fracture toughness, $K_{IC}$/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 \[19\]:

$$K_{IC} = \frac{\varepsilon_f n^2 E R_m}{60}$$  \hspace{1cm} (9)

where $\varepsilon_f$ is the true fracture strain, $n$ is the strain-hardening exponent, $E$/MPa is the modulus of elasticity.

True fracture strain can be expressed by percent reduction of area, $Z\%$:

$$\varepsilon_f = \ln\left(1 - \frac{Z}{100}\right)^{-1}$$  \hspace{1cm} (10)

The strain-hardening exponent can be defined by:

$$\frac{R_m}{R_c} \left(\frac{Z}{0.002e}\right)^n = 0$$  \hspace{1cm} (11)

### 4. Prediction of tensile test results and fracture toughness distribution in workpiece of complex form

The established method is applied in prediction of mechanical properties of quenched and tempered steel shaft made of steel 42CrMo4 (EN).

The chemical composition of investigated steel is shown in Table 1. Jominy test results of steel 42CrMo4 (EN) are shown in Table 2. Geometry of steel shaft is shown in Figure 3. Parameters of heat treatment of shaft are shown in Table 3.

The as-quenched hardness distribution in the quenched and tempered steel shaft is shown in Figure 4. Hardness distribution in the quenched and tempered steel shaft is shown in Figure 5.

Critical location for crack growth are locations 1 and 2 (Figs. 3, 4 and 5). Mechanical properties in critical locations of quenched and tempered steel shaft for tempering at 480°C are shown in Table 5.

### Table 1. Chemical composition of steel 42CrMo4 (EN)

<table>
<thead>
<tr>
<th>Chemical composition/wt.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
</tr>
<tr>
<td>0.38</td>
</tr>
</tbody>
</table>

### Table 2. Jominy test results of steel 42CrMo4 (EN)

<table>
<thead>
<tr>
<th>Jominy distance/mm</th>
<th>Hardness HRC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>55</td>
</tr>
<tr>
<td>3</td>
<td>54</td>
</tr>
<tr>
<td>5</td>
<td>54</td>
</tr>
<tr>
<td>7</td>
<td>53</td>
</tr>
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<td>9</td>
<td>51</td>
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<td>11</td>
<td>49</td>
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<td>25</td>
<td>35</td>
</tr>
<tr>
<td>30</td>
<td>33</td>
</tr>
</tbody>
</table>

### Table 3. Parameters of heat treatment of shaft

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Time</th>
<th>Media</th>
<th>Temperature</th>
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<th>Media</th>
</tr>
</thead>
<tbody>
<tr>
<td>850°C</td>
<td>1 hour</td>
<td>air</td>
<td>480°C</td>
<td>1 hour</td>
<td>air</td>
</tr>
</tbody>
</table>
Fig. 1. R-square for established algorithm (Eq. 1, Eq. 2)

Table 4.
Mechanical properties in critical locations of quenched and tempered steel shaft

<table>
<thead>
<tr>
<th>Properties</th>
<th>Critical location in Figures 3, 4 and 5</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Hardness HV</td>
<td>383</td>
</tr>
<tr>
<td>Tensile strength $R_m$ N/mm$^2$</td>
<td>1264</td>
</tr>
<tr>
<td>Yield strength $R_y$ N/mm$^2$</td>
<td>1067</td>
</tr>
<tr>
<td>Percent elongation $A$ %</td>
<td>8.6</td>
</tr>
<tr>
<td>Percent reduction of area $Z$ %</td>
<td>49.3</td>
</tr>
<tr>
<td>Fracture toughness $K_{IC}$ MPa m$^{1/2}$</td>
<td>107</td>
</tr>
</tbody>
</table>
Analysis and modelling

Computer simulation of quenched and tempered steel properties

Fig. 3. Geometry of steel shaft

Fig. 4. Hardness distribution in as-quenched steel shaft

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</tr>
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</tr>
</tbody>
</table>
5. Conclusions

A mathematical model for prediction of hardness in quenched and tempered steel workpiece is presented. In proposed model material properties and parameters of heat treatment should be taken into account.

A developed mathematical model has been applied in computer simulation of a quenched and tempered steel shaft. The computer simulation is based on finite volume method. The as-quenched 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. Hardness of the quenched and tempered workpiece is predicted based on as-quenched hardness and temperature of tempering. The prediction of distribution of yield strength is based on steel hardness distribution.

Based on experimental verification it could be concluded that mechanical properties of quenched and tempered steel workpieces can be calculated by the proposed method.

References


