Computer Simulation of Microstructure Transformation during the Quenching

B. Smoljan

Faculty of Engineering, Chair of Materials Science and Engineering
Vukovarska 58, 51000 Rijeka, Croatia

ABSTRACT:

Computer simulation of austenite decomposition during the steel quenching has been investigated.

The inversion method of phase portion estimation in the quenched steel has been established. The method of prediction of quenched steel microstructure composition is based on hardenability curve of Jominy-specimen.

The designed method of prediction austenite decomposition has been used in computer simulation of phase portion vs. hardness in quenched specimens of steel 34 Cr 5 and C 45 (DIN).

KEYWORDS: Austenite decomposition, Computer simulation

1 INTRODUCTION

Simulation of phase transformation is in the root of the simulation steel quenching. A model of quenching would not be considered representative of the actual process if it does not incorporate the effects of phase transformations. Phase transformation modeling is one of the main challenges in modeling of heat treatment [1].

Simulation of any one process can be made successfully only if all mechanisms of process are well known and if the appropriate mathematical methods are used. Unfortunately the mechanism of phase transformations is not fully understood and interactive influence of different elements, austenitizing temperature, etc. usually are not taken in account. The errors in phase transformation calculation could be extremely great if a model is based only on grain size of prior austenite, austenitizing temperature and elemental composition of steel. Phase transformation kinetic depends also on the degree of solution of the carbides and it cannot be accurately predicted only from elemental composition. The grain size at the austenitizing temperature must be known in calculation of phase transformation kinetic. Moreover, in practice numerous phase transformations calculations are based just on statistic correlation between chemical composition and final microstructure as result of quenching.

The investigations of steel quenching suggests that choosing a proper representative of the cooling phenomenon, which is relevant for structural transformation is one of the most important factors for a good simulation of hardening [2].

Good results in phase transformations prediction could be achieved if the prediction is based on continuous cooling transformations diagrams (CCT diagrams) [3]. CCT diagrams are irreplaceable
in the clear presentation of structural transformation during the steel cooling in order to predict structural constitution and hardness after cooling. Moreover, preparing CCT diagrams is rather expensive. They are prepared for strictly determined elemental composition and austenitizing temperature and they could be used with accuracy only for simulation of steel quenching with same elemental composition, austenitizing temperature and history as were of steel for it the CCT diagram is made. The computation of CCT diagrams upon the elemental composition has not been sufficiently developed.

From another point of view, the kinetic of phase transformations can be estimated based on simple experiment. For example, the kinetic of phase transformations and hardness distribution can be estimated based on time, relevant for structure transformation measured on Jominy specimen [4].

2 ALGORITHM OF PHASE PORTION PREDICTION

Structure composition after cooling is depended of on actual steel hardness. It can be written that the steel hardness generally is equal:

$$HV=\left(\% \text{ ferrite} \ HV_{(F)} + (\% \text{ pearlite}) \ HV_{(P)} + (\% \text{ bainite}) \ HV_{(B)} + (\% \text{ martensite}) \ HV_{(M)} \right)/100$$  (1)

In addition, the all amount of phases portion is equal unity:

$$(\% \text{ ferrite} + \% \text{ pearlite} + \% \text{ bainite} + \% \text{ martensite}) / 100 = 1$$  (2)

By the equations (1) and (2) is not difficult to predict phase fractions. Both, hardness (HV) of cooling microstructure with 90% or 50% of martensite and of 10%, 50% or 90% of (ferrite+pearlite), and hardness of microstructure constituents separately have to be known.

Results of austenite decomposition are depending 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 of cooling from 800 to 500 °C (time $t_{85}$) [4]. Involving the time $t_{85}$ in the mathematical model of steel quenching, the Jominy-test result can be involved in austenite decomposition model.

Everyone location of Jominy-sample has one characteristic time $t_{85}$. The diagram cooling time $t_{85}$ vs. distance from the quenched end of Jominy-specimen (Jominy-distance) is shown in Figure 1 [4].
If other heat treatment parameters are constant, the austenite decomposition results in some location of a cooled specimen will depend only of the time $t_{8/5}$.

It could be written for Jominy test that phase hardness depends of chemical composition ($CC$) and cooling rate parameter ($CRP$) that corresponds to actual distance ($d$) of Jominy specimen quenched end. It was adopted that $CRP = \log t_{8/5}^d$.

\[
HV_d^M = f_M(CC, CRP) = HV_{max}^M - K_M \log \frac{t_{8/5d}^M}{t_{8/5max}^M};
\]  
(3)

\[
HV_d^B = f_B(CC, CRP) = HV_{max}^B - K_B \log \frac{t_{8/5d}^B}{t_{8/5max}^B};
\]  
(4)

\[
HV_d^{P+F} = f_{P+F}(CC, CRP) = HV_N^{P+F} + K_{P+F} \log \frac{t_{8/5SN}^{P+F}}{t_{8/5d}^{P+F}};
\]  
(5)

where $N$ is normalizing, $B_{max}$ is lower bainite. Characteristic value of $HV$, $K$ and $t_{8/5}$ in equations (3), (4) and (5) has to be evaluated based on chemical composition for investigated steel combined by Jominy test results.

Hardness of quenched structures with 100%, 90% or 50% of martensite can be predicted by using the diagram of hardness at different percentages of martensite vs. carbon content after Hodge and Orehoski [1][5] and Jominy curve, but the influence of chemical composition of steel has to be taken in account.

Distances of quenched end Jominy specimen with martensite fraction of 90% and 50% can be predicted by the diagram of Jominy curve by conversion hardness results to distances.
Distances of 100% martensite and 100% of pearlite can be predicted by the diagram of Jominy curve.

The regression relations between the cooling time from 800 to 500°C for cooling structures of 100%, 50%, 10% and 0% pearlite are established.

\[
\log \left( \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{90\%(P+F)}} \right) = f_{90}(CC, T_a, t_a); \\
\log \left( \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{50\%(P+F)}} \right) = f_{50}(CC, T_a, t_a); \\
\log \left( \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{10\%(P+F)}} \right) = f_{10}(CC, T_a, t_a); \\
\log \left( \frac{t_{8/5}^{100\%(P+F)}}{t_{8/5}^{0\%(P+F)}} \right) = f_0(CC, T_a, t_a);
\]

where \( T_a \) is austenitizing temperature in K; \( t_a \) is austenitizing time in h;

Characteristic Jominy distances for characteristic time \( t_{8/5} \) is estimated using the relation between cooling time and distance from the quenched end of Jominy specimen shown in Figure 1.

### 3 COMPUTER SIMULATION OF PHASE PORTION

The phase portion of Jominy specimen of steel 34 Cr 4 (DIN) and C 45 (DIN) are estimated by computer simulation. An own computer software program was used for computer simulation.

Elemental composition of investigated steel 34 Cr 4 was 0.36% C, 0.28% Si, 0.63% Mn, 1.15% Cr. Jominy test results of investigated steel 34 Cr 4 are shown on Figure 3. Austenitizing temperature was equal 850 °C.
Diagram of structure portion for Jominy specimen of steel 34 Cr 4 is shown on figure 4.

Elemental composition of investigated steel C45 was 0.44% C, 0.28% Si, 0.60% Mn. Jominy test results of investigated steel C45 are shown on Figure 5. Austenitizing temperature was equal 850 °C.
Diagram of structure portion for Jominy specimen of steel C45 is shown on figure 6.

If the hardness in quenched specimen points is known and if the phase distribution vs. Jominy distances is known it is not difficult to predict the phase distribution in quenched steel specimen. Phase distribution in quenched steel specimen can be calculated by numerical methods [6] from time $t_{85}$ or by empirical methods using the diagram on figure 1 and Crafts - Lamont diagrams [5].
The calculated hardness distribution and phase distribution in quenched cylindrical steel specimen of 50 mm Dia. of steel C 45 is shown on figure 7. Heat treatment of quenching was: heating to 850 °C for 30 min and quenching in agitated water with severity of quenching H=1.4.

![Graph showing hardness distribution and phase proportion](image)

**Fig. 7** Simulated structure composition of cylindrical specimen of steel C45.

### 4 CONCLUSION

Simulation of phase transformation is in the root of the simulation steel quenching. A model of quenching would not be considered representative of the actual process if it does not incorporate the effects of phase transformations. Phase transformation modeling is one of the main challenges in modeling of heat treatment.

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 of cooling from 800 to 500 °C (time $t_{8/5}$).

The inversion method of computer simulation of austenite decomposition and evaluation of quenched phase portion was established. In the established mathematical model the numerical measure of specimen cooling kinetic was time $t_{8/5}$. For the calculation of microstructure composition, the hardness in specimen points, *Jominy* test results and chemical composition of steel must be known.

The established mathematical model was applied in computer simulation of microstructure transformation in *Jominy* and cylindrical specimens of steel. It can be concluded, that by proposed method microstructure composition in quenched steel specimen can be successfully calculated.
REFERENCES